# RIVM ZZS-2-BIO project

## The biobased replacement potential of hazardous substances.

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Report 1506

**Colophon**


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## Abstract

A quick scan of the ZZS (zeer zorgwekkende stoffen) list of 371 substances of very high concern shows that there is significant potential in biobased replacement of part of the list. Most inorganic (i.e. metal based or metal containing) substances on the list cannot be replaced by biobased (or fossil based) alternatives due to their specific physical/chemical properties or applications; e.g. the use of arsenic in solar cells or the use of lead oxide in glass manufacturing.

Some ZZS substance categories are very complex, requiring more time and effort to analyse; such as the petroleum products, but also the coal tar products. Since these categories deal with very large volumes, changes in particular components of integrated chains have impact on the total chain, and hence should be treated with care. A detailed analysis of these complex substance categories thus falls outside of the scope of this quick scan. They could, however, be the subject of a new, dedicated study.

For the remaining part of the substances of very high concern it is shown that in many cases easily implementable biobased alternatives are already available or in advanced stages of development. However, in some cases safe, biobased alternatives are still in early development. This in spite of a growing need for replacement, as is the case for e.g. high polarity aprotic solvents such as DMF, or NMP. Since solvents like NMP enable the manufacturing of environmentally friendly water borne coatings and paints, as well as the development of various carbohydrate based materials, finding effective substitutes should be given high priority. Unfortunately, currently there are no Dutch national science programs that could support or initiate this.

Also more advanced, indirect type of replacement appears feasible. An example of possible short term implementation is the partial replacement of toxic ethylene oxide for the production of ethylene glycol by the hydrogenolysis of glucose to ethylene glycol and propylene glycol. Other advanced level replacements require more time, and deeper analysis in order to assess the impact on product/value chains.

A shortlist of nine substances that could be replaced by biobased alternatives on short term is also presented in this quick scan report. The suggested biobased alternatives for this shortlist are either already commercially available or close to commercialisation.

Overall, this quick scan results in a number of recommendations

- A dedicated follow-up study into the biobased replacement potential for the petroleum products and coal tar products categories.
- Investigate the possibilities for a program on alternative, preferentially biobased, high polarity solvents that can involve the whole value chain, from production to specific applications.
- Specific follow-up studies on ZZS substances for which advanced level replacements have been identified (mid to long term replacements)
- Start a discussion between end-users of the substances on the shortlist, and (potential) producers of biobased alternatives, in order to evaluate the practical feasibility of biobased substitution.

**Content**



# 1 Introduction

Given the transnational scope of the subject (inventory of chemical substances of very high concern in the EU), combined with the fact that most information on these substances can be found in non-Dutch databases, the language of this report is English. Nevertheless, various terms and descriptions will remain in Dutch.

The policy on chemical substances by the Dutch Ministry of Infrastructure and Environment (Min. I&M) sets targets for reducing the exposure of both man and environment to dangerous chemical substances, particularly for substances called 'zeer zorgwekkende stoffen' (ZZS). These substances are defined by criteria stated in article 57 of the European REACH Regulation and taken up in the respective REACH and CLP Annexes as Substances of Very High Concern (SVHC). In addition, the Ministry considers substances that are listed as 'priority hazardous' in the European Water Framework Directive, the European POP Regulation or within the OSPAR convention as ZZS as well, as these fulfill the criteria stated in article 57.f for substances with an 'equivalent level of concern'. So SVHCs as taken up in the annexes of REACH and CLP as well as (other) substances that fulfill the criteria of article 57.f are referred to as ZZS.
These substances are identified at European level and depending on the nature, application and use volumes, measures are being taken to achieve a gradual phase-out. This phase-out has already begun for certain substances, such as certain types of phthalate plasticisers that have been put on the annex XIV list of the REACH regulation. The use of these substances is prohibited from a certain date, unless companies request an authorisation for use. From a policy perspective it is not only desirable to support the ongoing processes at European level, but also, where possible, to stimulate Dutch enterprises to replace substances of very high concern pro-actively.

Substitution can be achieved in various ways. In the search for functional substitutes to substances of very high concern, increasingly the potential of biobased alternatives is included. The development of a renewable feedstock based chemical industry is an ongoing process. The transition of a fossil resource to a biobased chemical industry offers opportunities for an accelerated phase-out of substances of very high concern. In order to effectively exploit these opportunities supply of biobased alternatives and demand for safe substitutes for substances of very high concern need to be matched, i.e. companies from the supply and demand side need to be brought into contact. The goal of this project is to perform a quick scan matching initiatives from the biobased chemical industry with (groups of) substances of very high concern, whose substitution is highly desirable. The outcome of this quick scan will serve as an important source of information for a symposium to be held at the beginning of 2015. The quick scan will list the most important examples of substitution of substances of very high concern by biobased products or processes as well as chances for developments in the Netherlands.

In 2013 the RIVM published a report named "Biobased alternatieven voor prioritaire stoffen: Een verkennende studie".[1] This study is a basic inventory of biobased alternatives for existing chemicals in the Netherlands which are currently available or being developed. Although several dozen substances were identified in this report, the list is not exhaustive. The report furthermore gives an overview of available methodologies to assess health and safety risks as well as the sustainability of (new) biobased substances, since biogenic substances are not necessarily safer or more sustainable than fossil derived ones. The current quick scan report is a continuation, in higher detail, of the aforementioned 2013 study.

# 2 Methods

The information on usage/application of the chemicals of high concern is obtained from internet searches using Google, Wikipedia and specific websites of companies, either producers or end-users of the chemicals. Also public information retrievable from e.g. the European Chemicals Agency (ECHA) and the US Environmental Protection Agency (EPA) website has been used. Information on tonnage is based on the data supplied by the RIVM as available from publically disseminated REACH registrations.

The use of patent literature for this study is limited due to several factors. Patent (applications) can be an indication that the assignees (companies or institutes) are active in a certain field of innovation, but can also be used defensively, e.g. to generate freedom to operate, or to divert attention from actual developments. Furthermore, often commercially important developments are not patented in early stages in order to prevent premature public dissemination of knowledge. While for some specific developments patent searches can be done with relative ease, more generic searches or searches involving broadly applicable chemicals can be highly time consuming. E.g. the subject ethylene oxide (oxirane) already gives 1.528 hits in the Espacenet database over the period 2000-2014. Hence, finding relevant patent literature for the 371 substances under consideration in this report falls outside of the scope of the current project.

In this study the chemicals under investigation are part of a list of 371 substances of very high concern as given by the RIVM.

In order to structure the information the data are presented as follows in table form:

- the name (as given in the RIVM list), as well as other, more commonly recognised names
- the CAS# number
- the type of compound:
  - Intermediate for substances that are commonly transformed into other products, and are not significantly applied in end-products
  - Solvents
  - Additives
  - Minerals
  - Ores
  - Pesticides
  - Catalysts
- Classification as either organic (Org) or inorganic (Inorg)
- BR-level: biobased replacement level (see below)
- When applicable/desirable the chemical structure is given
- Major applications/markets
- Biobased options/(potential) Suppliers/Stakeholders
  - Company names are anonymised, designated as CMP#, while trade/product names are anonymised as TP#.

# 3 Results & Discussion

For most of the substances on the ZZS list (see table 1), only those that are registered in the scope of the REACH Regulation with a reported tonnage of > 100 ton per year are discussed. The reported tonnages are the total annual European registration volumes, i.e. production and import into the EU.

In this report a biobased replacement level (or BR-level) is introduced, which serves as an indication for the potential for replacement of a substance of high concern by biobased alternatives.
The four different BR-levels used in this report are defined as:

- Level 0: no known possibilities either at the current state of technological development or due to the inherent chemical/physical properties/requirements.
- Level 1: drop-in replacement
    - drop-in is useful only in case the toxicity of the substance of high concern is due to (a) contaminant(s) (e.g. benzene) in the product that arise from the currently used feedstocks and/or conversion technologies, which can be eliminated by using an alternative feedstock.
- Level 2: direct replacement of the substance of high concern by a biobased alternative, based on comparable functionality.
    - Example: replacement of phthalate plasticisers by biobased non-phthalate plasticisers.
- Level 3: indirect replacement of substance of high concern.
    - More complex, probably longer term process, as it involves biobased replacement of the material that the substance of high concern is used in.

Since most biobased materials are by definition organic substances (apart from minerals like e.g. silica that can be obtained from agroresidues), the focus is on these type of substances on the ZZS list.

On short term (1-5 years) only level 1 and level 2 replacements are feasible as they will have the smallest impact on the whole product/value chain. Level 1 replacement will require minimal changes in the production chain, as the drop-in substance will be practically similar to the original substance. Level 2 replacement will require investments in redesigning chemical processes or processing conditions, re-formulating, and end-product testing (e.g. quality, durability, functionality, toxicity, stability, flammability, etc.). Of course care must be taken that a biobased level 2 replacement is inherently safe.
Level 3 replacement is even more complex since it involves redesigning the product/value chain. Care must be taken to exclude unwanted side effects, like overall reduction of efficiency or increase of unwanted emissions over the whole chain. These prerequisites of course also apply to level 1 and 2 replacements.

In this chapter only those substances that have a potential for biobased replacement (BR levels 1-3) will be discussed. The remaining substances, identified with BR level 0, are listed in the appendix. These substances have no biobased replacement options due to inherent properties. In case of the inorganic substances, the inherent/required chemical or physical properties fall outside of the scope of organic substances (e.g. mercury, cadmium salts, etc). In case of BR level 0 organic substances, the current applications are too specific (inherent chemical properties) to allow for (biobased) replacement.

Table 1: overview of the substances/substance groups discussed in this report.

| *Entry* | *Substance group* | *# ZZS registered Substances* | *# on Annex XIV candidate list* | *Org/Inorg* | *# Biobased replacement options* |
|---|---|---|---|---|---|
| **1** | Petroleum products | 219 | - | Org | nd |
| **2** | Other | 33 | 15 | Org | 12 |
| **3** | Lead/lead compounds | 26 | 26 | Org/Inorg | 4 |
| **4** | Nickel/nickel compounds | 15 | - | Inorg | 0 |
| **5** | Coal products | 13 | 2 | Org | >1 |
| **6** | Boron/boron compounds | 10 | 5 | Inorg | 0 |
| **7** | Cadmium/cadmium compounds | 6 | 4 | Inorg | 0 |
| **8** | Br/Cl hydrocarbons | 6 | 3 | Org | 1 |
| **9** | Oxiranes | 5 | 1 | Org | 3 |
| **10** | Chromium/chromium compounds | 4 | 4 | Inorg | 0 |
| **11** | Cobalt/cobalt compounds | 4 | 4 | Inorg | 0 |
| **12** | Phthalates | 3 | 3 | Org | 3 |
| **13** | Azo dyes | 3 | 3 | Org | 0 |
| **14** | Hydrazines | 3 | 2 | Inorg | 0 |
| **15** | Butadiene(s) | 3 | - | Org | 1 |
| **16** | Beryllium | 2 | - | Inorg | 0 |
| **17** | Brominated flame retardants | 2 | 1 | Org | 0 |
| **18** | Chlorinated aromatics | 2 | 1 | Org | 1 |
| **19** | Glycol ethers | 2 | 2 | Org | 2 |
| **20** | Organo mercury | 2 | - | Inorg | 0 |
| **21** | Non-approved PPP | 2 | 1 | Org | 0 |
| **22** | Phenols | 1 | 1 | Org | 0 |
| **23** | Arsenic compounds | 1 | - | Inorg | 0 |
| **24** | Organotin | 1 | 1 | Org | 1 |
| **25** | Acrylamide | 1 | 1 | Org | 0 |
| **26** | Dimethylformamide | 1 | 1 | Org | 1 |
| **27** | Formamide | 1 | 1 | Org | 0 |
| | **Total** | **371** | **82** | | **>29** |

### *Petroleum and coal products; entry 1 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 1 | Petroleum and coal products | 219 | - |

The extensive group of ZZS registered petroleum and coal-based products is too complicated to be discussed in detail in this quick scan. Most, if not all of these substances are part of the crude oil and coal distillation/fractionation process as applied by various oil companies or petrochemical processors. Crude oil distillation produces a large number of fractions/products, which form an integrated/interdependent family of substances. Changes in the production or use of certain fractions/product groups has direct impact on the whole system making this rather complex. Furthermore, due to the very large scale of operations, even small changes can have dramatic impact. The overall economy of the distillation process depends on complete valorisation of the feedstock. Taking out fractions will hence also have significant impact on the economic viability of the whole process. An investigation into potential biobased replacement of substances in the petroleum/coal products group therefore requires dedicated attention, and warrants a separate specific project.

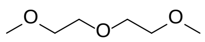
 

## *Other; entry 2 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 2 | Other | 33 | 15 |

The category "other" contains a list of 33 substances of various types (in the original ZZS list order), with widely differing applications and tonnages.Out of this category 12 substances have been selected as having BR level 2, or 3 and are discussed below.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| bis(2-methoxyethyl) ether, diglyme | 111-96-6 | Solvent | | 100-1,000 | Org | 2 |



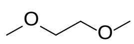
**Applications/Markets**

High boiling, high polarity solvent.

**Biobased options/(potential) Suppliers/Stakeholders**

Several biobased ethers and esters are possible: isosorbidedimethyl ether (CMP1), lactic acid esters (CMP2, CMP3), glycerol ethers, γ-valerolactone (CMP4), methyl levulinate (ML, CMP4), 2-methyl-THF.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 1,2-dimethoxyethane; ethylene glycol dimethyl ether; glyme (EGDME) | 110-71-4 | Solvent | | 100-1,000 | Org | 2 |



**Applications/Markets**

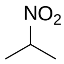
Together with a high-permittivity solvents (e.g. propylene carbonate), dimethoxyethane is used as the low-viscosity component of the solvent for electrolytes of lithium batteries. Dimethoxyethane is also a good solvent for oligo- and polysaccharides.

**Biobased options/(potential) Suppliers/Stakeholders**

Glymes are amongst others produced by CMP5.
Several biobased ether are possible: isosorbidedimethyl ether (CMP1), lactic acid esters (CMP2, CMP3), glycerol ethers, γ-valerolactone (CMP4), methyl levulinate (CMP4), 2-methyl-THF.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 2-nitropropane | 79-46-9 | Intermediate Solvent | | 1,000-10,000 | Org | 2 |




**Applications/Markets**

Chemical intermediate, solvent, inks, coatings, adhesives, polymers

**Biobased options/(potential) Suppliers/Stakeholders**

In its role as high polarity solvent 2-nitropropane could be replaced by high polarity biobased solvents like isosorbidedimethyl ether (CMP1), lactic acid esters (CMP2, CMP3), γ-valerolactone (CMP4), methyl levulinate (CMP4).

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| ethyleneimine; aziridine | 151-56-4 | Intermediate | | 100+ | Org | 3 |


**Applications/Markets**

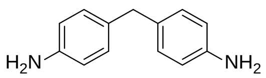
Ethyleneimine is used in polymerization products; as a monomer for polyethyleneimine (PEI); as a comonomer for polymers (e.g., with ethylenediamine); and in paper and textile chemicals, adhesives, binders, petroleum refining chemicals, fuels and lubricants, coating resins, varnishes, lacquers, agricultural chemicals, cosmetics, ion exchange resins, photographic chemicals, and surfactants. PEI finds many applications in products like: detergents, adhesives, water treatment agents and cosmetics. Thanks to the ability to modify the surface of cellulose fibres, PEI is employed as a wet-strength agent in the paper-making process.

**Biobased options/(potential) Suppliers/Stakeholders**

Biobased alternatives for PEI are under development and could reduce the need for ethyleneimine. The scope is too broad to give specific examples.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Formaldehyde, oligomeric reaction products with aniline (technical MDA) | 25214-70-4 | Intermediate | | 100-1,000 | Org | 2 |



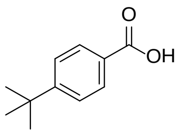

**Applications/Markets**

Technical MDA is registered as intermediate, mainly for the manufacture of methylene diphenyl diisocyanate (MDI). In addition to the use in the manufacture of MDI, the Annex XV report indicates the following uses for technical MDA:
- as curing agent for epoxy resins in
- in the production of high performance polymers
- as a starting point for the synthesis of 4,4'-methylenebis (cyclohexaneamine)

**Biobased options/(potential) Suppliers/Stakeholders**

Biobased diamines. However, most of these are aliphatic (other reactivity) and/or less rigid, giving different properties of the final product. Potential suppliers are CMP6, CMP7, CMP8.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 4-tert-butylbenzoic acid (PTBBA) | 98-73-7 | Intermediate | | 100-1,000 | Org | 2 |



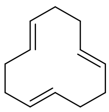
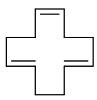
**Applications/Markets**

PTBBA is mainly used in the EU for the manufacture of thermal stabilisers in PVC. For this purpose, PTBBA is first converted into its metal salts (Metal-p-tert-butylbenzoate, Me-PTBB). According to ESPA (European Stabiliser Producers Association) six plants are using PTBBA for the production of liquid mixed metal stabilisers.[3]
The second most important use of PTBBA in the EU is the use as process regulator (chain stop agent) in polymers industry for producing alkyd and polyester resins.

**Biobased options/(potential) Suppliers/Stakeholders**

Potentially, lignin derived benzoic acid derivatives; these are however not yet commercial, while the eco-toxicological impact is still mostly unknown.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Cyclododecatriene (CDT) | 676-22-2, 706-31-0 | Intermediate | | Conf. | Org | 3 |

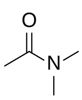
**Applications/Markets**

Chemical intermediate (butadiene trimerisation), precursor for dodecanedioic acid (antiseptics, coatings, corrosion inhibitor, surfactant, engineering plastics; PA12X), laurolactam (precursor to the polyamide PA12).

**Biobased options/(potential) Suppliers/Stakeholders**

For the end-application, high performance polyamides for e.g. automotive applications several biobased alternatives are already commercially available: PA1010, PA1012 (CMP6, TP1), CMP9, castor oil based (sebacic C10). Also long-chain biobased diacids are available from companies like CMP1 and CMP8.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Dimethylacetamide (DMAc) | 127-19-5 | Solvent | | 10,000-100,000 | Org | 2 |



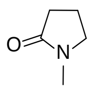
**Applications/Markets**

Dimethylacetamide is commonly used as a solvent for fibers (e.g., polyacrylonitrile, spandex) or in the adhesive industry. It is also employed in the production of pharmaceuticals and plasticizers as a reaction medium.

**Biobased options/(potential) Suppliers/Stakeholders**

There is a broadly recognised need for alternatives to polar aprotic solvents, like DMAc, DMF, and NMP. Significant efforts are being undertaken to develop effective, safe biobased alternatives. None are currently commercially available on large scale. Furthermore, no "one-size fits all" solutions have been found yet.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| N-Methyl-2-pyrrolidone (NMP) | 872-50-4 | Solvent, Intermediate | | 10,000-100,000 | Org | 2 |




**Applications/Markets**

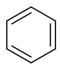
NMP is used to recover pure hydrocarbons while processing petrochemicals (such as the recovery of 1,3-butadiene using NMP as an extractive distillation solvent) and in the desulfurization of gases. Due to its good solvency properties N-methyl-2-pyrrolidone is used to dissolve a wide range of chemicals, especially in the polymers field. It also used as a solvent for surface treatment of textiles, resins and metal coated plastics or as a paint stripper. It is utilized as a solvent in the commercial preparation of polyphenylene sulfide. In the pharmaceutical industry, N-methyl-2-pyrrolidone is used in the formulation for drugs by both oral and transdermal delivery routes. NMP and its derivatives are used as intermediates for the synthesis of agrochemicals, pharmaceuticals, textile auxiliaries, plasticizers, stabilizers and specialty inks. It is also employed as a nylon precursor. The rubber industry uses it for SBR latex production and the electronics industry for printed circuit board manufacturing.

**Biobased options/(potential) Suppliers/Stakeholders**

There is a broadly recognised need for alternatives to polar aprotic solvents, like DMAc, DMF, and NMP. Significant efforts are being undertaken to develop effective, safe biobased alternatives. None are currently commercially available on large scale. Furthermore, no "one-size fits all" solutions have been found yet.
The paints and coatings industry is very interested in developing sustainable alternatives for NMP as dispersing agent in the production of water borne high solids coatings. These products have been developed as alternative to organic solvent borne coatings systems and the related problem of VOC emissions. The development of biobased water

borne high solids coatings also strongly depends on the use of dispersing agents like NMP, since many of the biobased coatings systems currently under development, like non-isocyanate polyurethanes (NIPU's), are chemically and structurally different from their petrochemical analogues (i.e. more polar) requiring high polarity solvents.

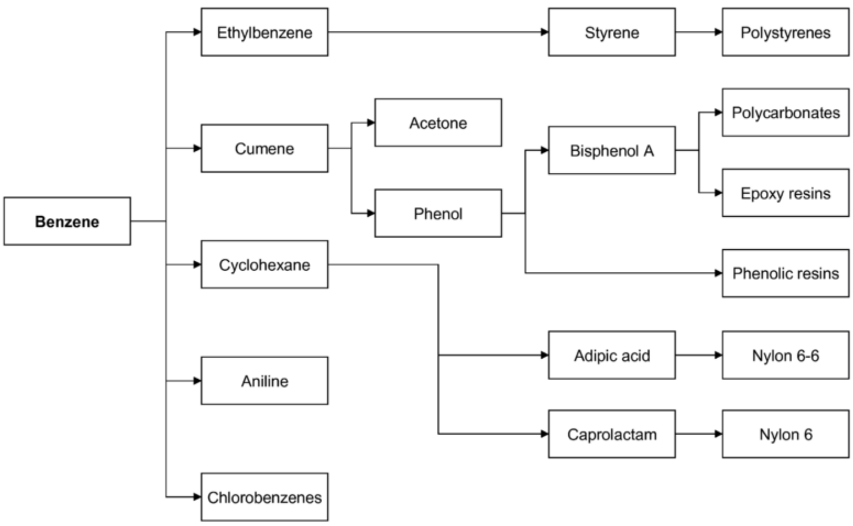
| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Benzene | 71-43-2 | Intermediate | | 1,000-10,000 | Org | 3 |



**Applications/Markets**

Benzene is used mainly as an intermediate to make other chemicals. About 80% of benzene is consumed in the production of three chemicals, ethylbenzene, cumene, and cyclohexane. Its most widely produced derivative is ethylbenzene, precursor to styrene, which is used to make polymers and plastics. Cumene is converted to phenol for resins and adhesives. Cyclohexane is used in the manufacture of Nylon. Smaller amounts of benzene are used to make some types of rubbers, lubricants, dyes, detergents, drugs, explosives, and pesticides.

In both the US and Europe, 50% of benzene is used in the production of ethylbenzene/styrene, 20% is used in the production of cumene, and about 15% of benzene is used in the production of cyclohexane (eventually to nylon).

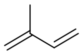



**Biobased options/(potential) Suppliers/Stakeholders**

Phenol and cyclohexane can be obtained from lignin, although these processes are still mainly at an academic stage.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Isoprene, 2-methyl-1,3-butadiene | 78-79-5 | Intermediate | | 10,000-100,000 | Org | 3 |



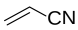
**Applications/Markets**

It is most readily available industrially as a by-product of the thermal cracking of naphtha or oil, as a side product in the production of ethylene. About 800,000 tonnes are produced annually. About 95% of isoprene production is used to produce cis-1,4-polyisoprene, a synthetic version of natural rubber.[2]

**Biobased options/(potential) Suppliers/Stakeholders**

Synthetic natural rubber is highly similar to natural rubber from *Hevea brasiliensis* (the rubber tree), but does not lead to allergic reactions due to the absence of residual proteins. Alternative sources of natural rubber like Russian Dandelion and Guayule could be an option in order to prevent *Hevea* specific latex allergies.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Acrylonitrile | 107-13-1 | Intermediate | | 1,000,000-10,000,000 | Org | 3 |



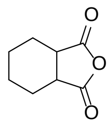

**Applications/Markets**

Most industrial acrylonitrile is produced by catalytic ammoxidation of propylene, also known as the Sohio process. Acrylonitrile is used principally as a monomer to prepare polyacrylonitrile (PAN) or several important copolymers, such as styrene-acrylonitrile (SAN), acrylonitrile butadiene styrene (ABS), acrylonitrile styrene acrylate (ASA), and other synthetic rubbers such as acrylonitrile butadiene rubber (NBR). PAN is the precursor for high strength carbon fiber. Dimerization of acrylonitrile affords adiponitrile, used in the synthesis of certain polyamides (PA66). Acrylonitrile is also a precursor in the industrial manufacture of acrylamide and acrylic acid. Acrylamide is prepared on an industrial scale by the hydrolysis of acrylonitrile by nitrile hydratase. Most acrylamide is used to synthesize polyacrylamides(PAM), which find many uses as water-soluble thickeners. These include use in wastewater treatment, papermaking, ore processing, tertiary oil recovery, and the manufacture of permanent press fabrics.

**Biobased options/(potential) Suppliers/Stakeholders**

Biobased options are only partially feasible at level 3 replacement, which are long term developments, e.g. in the area of biobased carbon fibers, or polysaccharide based thickeners (CMP10, CMP11, CMP12).

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Cyclohexane dicarboxylic anhydride, Hexahydrophthalic anhydride, HHPA | 85-42-7 | Intermediate | | 10,000-100,000 | Org | 2 |




**Applications/Markets**

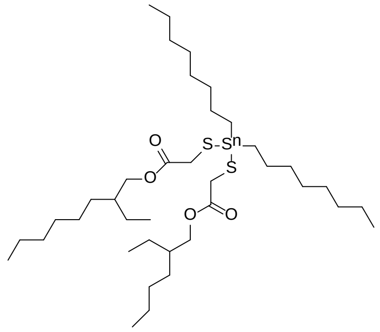
Anhydride curing agent for aliphatic epoxy resins. Intermediate for expoxy resins. Low viscosity reactive diluents. The low viscosity and high latency of anhydride hardeners makes them suitable for processing systems which require addition of mineral fillers prior to curing, e.g. for high voltage electrical insulators. Intermediate for PVC plasticisers. Unsaturated polyester resin co-monomer, intermediate for alkyd resins and rust inhibitors.

**Biobased options/(potential) Suppliers/Stakeholders**

Several level 2 biobased alternatives can be thought of, such as itaconic anhydride, (methyl)succinic anhydride (CMP13) and Diels-Alder adducts from furan and maleic anhydride.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| di-n-Octyltin-bis-2-ethylhexyl-mercaptoacetate | 15571-58-1 | Additive | | 1,000-10,000 | Inorg/Org | 2 |




**Applications/Markets**

Liquid tin PVC stabilizer.

**Biobased options/(potential) Suppliers/Stakeholders**

Level 2 replacement involves development of organic, biobased PVC heat stabilisers, such as dihydropyridines or uracils. Stakeholders are e.g. CMP14, CMP15, CMP16, CMP17, CMP18, CMP19.

## *Lead/lead compounds; entry 3 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 3 | Lead/lead compounds | 26 | 26 |

The list of lead compounds contains many inorganic substances that serve as intermediate for glass and ceramics production and lead battery production (see appendices). Those lead compounds that are eligible for biobased replacement fall under the category PVC heat stabilisers. Lead stabiliser phase out is to be finalised in the EU by 2015. Whereas most lead based stabilisers are being replaced by calcium/zinc stabilisers, development of organic biobased stabilisers is still interesting from a sustainability perspective.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Dioxobis(stearato)trilead, Dibasic lead stearate (DBLS) | 12578-12-0 | Additive | | 100,000-1,000,000 | Inorg/Org | 2 |

**Applications/Markets**

Di Basic Lead Stearate finds application in cable manufacturing, PVC processing, calandering operations and extrusions. Due to toxicity, Di Basic Lead Stearate is not used in articles that are likely to come in contact with foodstuff. Normally, Di Basic Lead Stearate is used along with Lead Stearate and Tri Basic Lead Sulphate.

**Biobased options/(potential) Suppliers/Stakeholders**

Level 2 replacement involves development of organic, biobased PVC heat stabilisers, such as dihydropyridines or uracils. Stakeholders are e.g. CMP14, CMP15 , CMP16, CMP17, CMP18, CMP19.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Fatty acids, C16-18, lead salts | 91031-62-8 | Additive | | 10,000-100,000 | Inorg/Org | 2 |

**Applications/Markets**

PVC stabiliser, lubricants.

**Biobased options/(potential) Suppliers/Stakeholders**

Level 2 replacement involves development of organic, biobased PVC heat stabilisers, such as dihydropyridines or uracils.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Sulfurous acid, lead salt, dibasic | 62229-08-7 | Intermediate | | 100-1,000 | Inorg | 2 |

**Applications/Markets**

Intermediate for PVC stabilisers.

**Biobased options/(potential) Suppliers/Stakeholders**

Level 2 replacement involves development of organic, biobased PVC heat stabilisers, such as dihydropyridines or uracils. Stakeholders are e.g. CMP14, CMP15 , CMP16, CMP17, CMP18, CMP19.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Trilead dioxide phosphonate (Dibasic Lead Phosphite) | 12141-20-7 | Additive | | 100,000-1,000,000 | Inorg | 2 |

**Applications/Markets**

PVC stabilizer.

**Biobased options/(potential) Suppliers/Stakeholders**

Level 2 replacement involves development of organic, biobased PVC heat stabilisers, such as dihydropyridines or uracils. Stakeholders are e.g. CMP14, CMP15, CMP16, CMP17, CMP18, CMP19.

## *Nickel/nickel compounds; entry 4 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 4 | Nickel/nickel compounds | 15 | - |

None of the nickel compounds mentioned on the ZZS list is eligible for biobased replacement due to very specific intrinsic properties of these metal containing substances.

## *Coal products; entry 5 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 5 | Coal products | 13 | 2 |

The terms tar and pitch are often used interchangeably. However, pitch is considered more solid while tar is more liquid. Coal tar is a brown or black liquid of extremely high viscosity. Coal tar is among the by-products when coal is carbonized to make coke or gasified to make coal gas. Coal tars are complex and variable mixtures of phenols, polycyclic aromatic hydrocarbons (PAHs), and heterocyclic compounds. When used for many industrial processes, bituminous coal must first be "coked" to remove volatile components. Coking is achieved by heating the coal in the absence of oxygen, which drives off volatile hydrocarbons such as propane, benzene and other aromatic hydrocarbons, and some sulphur gases. This also drives off a considerable amount of the contained water of the bituminous coal. Coking coal is used in the manufacture of steel, where carbon must be as volatile-free and ash-free as possible.[2,4]

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Extract residues (coal), light oil alk., acid ext., indene fraction | 101316-62-5 | Intermediate | - | 10,000-100,000 | Org | ? |
| Tar acids, methylphenol rich in 3- and 4-methylphenol | 84989-04-8 | Intermediate | - | 1,000-10,000 | Org | ? |
| Tar, brown-coal, low-temp.; aliphatic, naphthenic and cyclic aromatic hydrocarbons, heteroaromatic hydrocarbons and cyclic phenols. | 101316-84-1 | Intermediate | - | 10,000-100,000 | Org | ? |
| Pitch, coal tar, high-temp., a complex mixture of three or more membered condensed ring aromatic hydrocarbons. | 121575-60-8 | Intermediate | - | 10,000-100,000 | Org | ? |
| Tar acids, xylenol fraction; rich in 2,4- and 2,5-dimethylphenol | 84989-06-0 | Intermediate | - | 1,000-10,000 | Org | ? |
| Solvent naphtha (coal), xylene-styrene cut | 85536-20-5 | Intermediate | - | 10,000-100,000 | Org | ? |
| Solvent naphtha (coal); indene and other polycyclic ring systems containing a single aromatic ring. | 65996-79-4 | Intermediate | - | 1,000-10,000 | Org | ? |
| Anthracene oil; | 90640-80- | Intermediate | - | 100,000- | Org | ? |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| complex combination of phenanthrene, anthracene and carbazole. | 5 | | | 1,000,000 | | |
| Creosote oil, acenaphthene fraction; acenaphthene, naphthalene and alkyl naphthalene. | 90640-84-9 | Intermediate | - | 100,000-1,000,000 | Org | ? |
| Distillates (coal tar), heavy oils; tri- and polynuclear hydrocarbons and heterocyclic compounds. | 90640-86-1 | Intermediate | - | 100,000-1,000,000 | Org | ? |
| Pitch, coal tar, high-temp.; complex mixture of three or more membered condensed ring aromatic hydrocarbons. | 65996-93-2 | Intermediate | - | 1,000,000-10,000,000 | Org | ? |
| Pyridine, alkyl derivs.; complex combination of polyalkylated pyridines derived from coal tar distillation. | 68391-11-7 | Intermediate | - | Conf. | Org | ? |

**Applications/Markets**

A Dutch based coal tar processor, CMP20, produces predominantly naphthalene, creosote, carbon black and pitch. The latter is used for the production of carbon electrodes, and also bitumen emulsions for road construction. The primary source of raw material is coal tar from steel mill cokes plants. As of 2012 the plant had a capacity to process 140,000 ton of tar per year.
A large part of the binders used in the graphite industry for making "green blocks" are coke oven volatiles (COV). A considerable portion of these COV used as binders is coal tar. During the baking process of the green blocks as a part of commercial graphite production [ e.g. electrodes for aluminium production], most of the coal tar binders are vaporised and are generally burned in an incinerator to prevent release into the atmosphere, as COV and coal tar can be injurious to health. Creosote was originally used as wood preservative. Coal tar is also used to manufacture paints, synthetic dyes, and photographic materials. Furthermore, coal tar distillates are a prime source of polyaromatic and heteroaromatic platform chemicals for fine chemical production. [2,4]

**Biobased options/(potential) Suppliers/Stakeholders**

Tar products can also be obtained from wood (wood-tar); which has a different composition. Various efforts are already being undertaken to replace creosote by biobased wood preservatives. Currently, there are no large scale commercial biobased alternatives.
Since coal tar distillates are complex mixtures of substances with various areas of applications it is difficult to assess the biobased replacement potential without detailed analyses of the value chains.
Biobased replacement levels could span from level 1, if drop-in replacement is free from e.g. PAHC contamination, to level 2 for e.g. creosote and level 3 for wood tar and activated carbon/graphite.

## *Boron/boron compounds; entry 6 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 6 | Boron/boron compounds | 10 | 5 |

None of the boron compounds mentioned in the ZZS list are eligible for biobased replacement due to the very specific intrinsic properties of these substances.

## *Cadmium/cadmium compounds; entry 7 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 7 | Cadmium/cadmium compounds | 6 | 4 |

None of the cadmium compounds mentioned in the ZZS list are eligible for biobased replacement due to the very specific intrinsic properties of these metal containing substances.

## *Br/Cl hydrocarbons; entry 8 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 8 | Br/Cl hydrocarbons | 7 | 3 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Alkanes, C10-13, chloro (Short Chain Chlorinated Paraffins) | 85535-84-8 | Additive | | 1,000-10,000 | Org | 2 |

**Applications/Markets**

Chlorinated paraffins are used as extreme-pressure-lubricant additives in metalworking fluids; as flame retardants in plastics, rubber, and paints; to improve water resistance of paints and fabrics; and as a secondary plasticizer in polyvinyl chloride.[2,5,6]

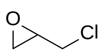
**Biobased options/(potential) Suppliers/Stakeholders**

For application as plasticiser several biobased alternatives are available or under development, e.g. isosorbide esters (CMP21), TP2(CMP22), citrate esters (CMP23). The suggested alternatives are only feasible in the role of plasticisers for PVC.

## *Oxyranes; entry 9 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 9 | Oxyranes | 5 | 1 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Epichlorohydrine, ECH | 106-89-8 | Intermediate | | 100,000-1,000,000 | Org | 3 |



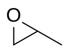

**Applications/Markets**

Epichlorohydrin is mainly converted to bisphenol A diglycidyl ether, a building block in the manufacture of epoxy resins. It is also a precursor to monomers for other resins and polymers.

**Biobased options/(potential) Suppliers/Stakeholders**

Biobased epoxides (non-BPA based) can be prepared via synthetic routes not involving ECH. There are currently no commercial products known. CMP9 and CMP24 produce biobased ECH from glycerol on small scale.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Propylene oxide | 75-56-9 | Intermediate | | 1,000,000 + | Org | 3 |



**Applications/Markets**

Between 60 and 70% of all propylene oxide is converted to polyether polyols for the production of polyurethane plastics. About 20% of propylene oxide is hydrolyzed into propylene glycol (unsaturated PE resins, de-icing), via a process which is accelerated by acid or base catalysis. Other major products are polypropylene glycol, propylene glycol ethers, and propylene carbonate.[10]

**Biobased options/(potential) Suppliers/Stakeholders**

Propylene glycol (PG), together with ethylene glycol (EG) can be prepared from biomass via hydrogenolysis of glucose (1st gen. from starch, 2nd gen. from cellulose) or glycerol. Various agro and chemical companies (e.g. CMP25, CMP3, CMP24) already produce bio EG and PG.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Ethylene oxide | 75-21-8 | Intermediate | | 1,000,000 + | Org | 3 |

**Applications/Markets**

Ethylene oxide is one of the most important raw materials used in the large-scale chemical production. Most ethylene oxide is used for synthesis of ethylene glycols, including diethylene glycol and triethylene glycol, that accounts for up to 75% of global consumption. Other important products include ethylene glycol ethers, ethanolamines and ethoxylates. Among glycols, ethylene glycol is used as antifreeze, in the production of polyester and polyethylene terephthalate (PET – raw material for plastic bottles), liquid coolants and solvents.

**Biobased options/(potential) Suppliers/Stakeholders**

The world's largest producers of ethylene oxide are CMP24 (3–3.5 million tonnes in 2006), CMP26 (1.328 million tonnes in 2008–2009) and CMP8 (1.175 million tonnes in 2008–2009).[12]

Propylene glycol (PG), together with ethylene glycol (EG) can be prepared from biomass via hydrogenolysis of glucose (1st gen. from starch, 2nd gen. from cellulose). Various agro and chemical companies (e.g. CMP25, CMP3, CMP27) already produce bio EG and PG. CMP27 and others however use a route via fermentation of sugar to bioethanol, dehydration to ethylene, and subsequently petrochemical methodology via ethylene oxide. So care must be taken to exclude bio EG obtained via this route since it still involves EO, and is energetically unfavourable.

## *Chromium/chromium compounds; entry 10 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 10 | Chromium/chromium compounds | 4 | 4 |

None of the chromium compounds on the ZZS list have potential for biobased replacement due to the very specific intrinsic properties of these metal containing substances.

## *Cobalt/cobalt compounds; entry 11 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 11 | Cobalt/cobalt compounds | 4 | 4 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Cobalt(II) diacetate | 71-48-7 | Catalyst | | 1,000 - 10,000 | Inorg | 2 |

**Applications/Markets**

Cobalt acetate is a precursor to various oil drying agents, catalysts that allow paints and varnishes to harden.

**Biobased options/(potential) Suppliers/Stakeholders**

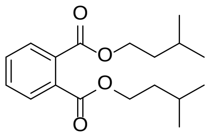
Cobalt acetate could be replaced by Iron/ascorbic acid (vitamin C) catalysts in some applications (still under development).

### *Phthalates; entry 12 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 12 | Phthalates | 3 | 3 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Diisopentylphthalate, isoamylphthalate | 605-50-5 | Additive, solvent | | 10-100 | Org | 2 |



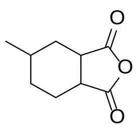
**Applications/Markets**

Not found.

**Biobased options/(potential) Suppliers/Stakeholders**

Could be e.g. replaced by isoamyl esters of furandicarboxylic acid (FDCA); not currently commercially available (CMP6, CMP3).

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Hexahydromethylphthalic anhydride | 25550-51-0 | Intermediate | | 1,000-10,000 | Org | 2 |
| Hexahydro-4-methylphthalic anhydride | 19438-60-9 | Intermediate | | 1,000-10,000 | Org | 2 |



**Applications/Markets**

Meythylhexahydrophthalic Anhydride (MHHPA) is produced by hydrogenation of Methyltetrahydrophthalic Anhydride (MTHPA), obtained by reacting isoprene with maleic anhydride. MHHPA is a thermo-setting epoxy resin curing agent mainly used in electric and electronic field. MHHPA has several advantages: Low melting point, low viscosity of the mixtures with alicyclic epoxy resins, long applicable period, high heat-resistance of the cured material and excellent electrical properties at high temperature. MHHPA is widely used for impregnating electrical coils, casting electricity components and sealing semiconductors, outdoor insulators, capacitors, light emitting diodes and digital displays.[2]

**Biobased options/(potential) Suppliers/Stakeholders**

Various possibilities exist for replacing these anhydrides by biobased aliphatic anhydrides; e.g. (methyl)succinic anhydride, itaconic anhydride, hexahydro-3-methylphthalic anhydride, etc. Some of these substances are commercially available on small scale, some are under development.

## *Azo dyes; entry 13 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 13 | Azo dyes | 3 | 3 |

These substances are low volume, very specific.

## *Hydrazines; entry 14 (>100 ton/annum)*

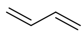
| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 14 | Hydrazines | 3 | 2 |

There are currently no biobased biobased alternatives for hydrazine due to very specific intrinsic properties of this substance.

## *Butadiene(s); entry 15 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 15 | Butadiene(s) | 3 | - |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 1,3-butadiene | 106-99-0 | Intermediate | | 10,000-100,000 | Org | 3 |



**Applications/Markets**

Most butadiene is polymerized to produce synthetic rubber. While polybutadiene itself is a very soft, almost liquid material, copolymers prepared from mixtures of butadiene with styrene and/or acrylonitrile, such as acrylonitrile butadiene styrene (ABS), acrylonitrile butadiene (NBR) and styrene-butadiene (SBR) are tough and/or elastic. SBR is the material most commonly used for the production of automobile tires.
Smaller amounts of butadiene are used to make the nylon intermediate, adiponitrile, by the addition of a molecule of hydrogen cyanide to each of the double bonds in a process called hydrocyanation developed by DuPont. Other synthetic rubber materials such as chloroprene, and the solvent sulfolane are also manufactured from butadiene. Cyclooctadiene and cyclododecatriene are produced via nickel- or titanium-catalyzed dimerization and trimerization reactions, respectively.

**Biobased options/(potential) Suppliers/Stakeholders**

Biobased replacement of cyclooctadiene and cyclododecatriene (see those specific entries) could reduce the need for butadiene for those applications

## *Beryllium; entry 16 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 16 | Beryllium | 2 | - |

No possibilities for biobased due to the very specific intrinsic properties of metallic substance.

## *Brominated flame retardants; entry 17 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 17 | Brominated flame retardants | 2 | 1 |

No possibilities for biobased due to the very specific intrinsic chemical properties i.e. the possibility to release bromine radicals under combustion conditions.

## *Chlorinated aromatics; entry 18 (>100 ton/annum)*

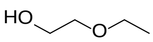
| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 18 | Chlorinated aromatics | 2 | 1 |

No possibilities for biobased, due to the very specific chemical functionality of these products. Functional biobased alternatives will probably have a comparably negative toxicological profile.

## *Glycol ethers; entry 19 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 19 | Glycol ethers | 2 | 2 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 2-ethoxyethanol; ethylene glycol monoethyl ether | 110-80-5 | Solvent | | 1,000-10,000 | Org | 2 |




**Applications/Markets**

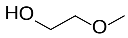
2-Ethoxyethanol, also known by the trademark Cellosolve or ethyl cellosolve, is a solvent used widely in commercial and industrial applications. 2-ethoxyethanol is used in products, such as varnish removers and degreasing solutions.[2,8]

**Biobased options/(potential) Suppliers/Stakeholders**

Methyl and Ethyl Cellosolve could be replaced by partially alkylated biobased di/triols, like trimethyl glycerol, tertiary butyl glycerol, monomethylisosorbide, etc. One of the few currently commercially available biobased alternatives are lactic acid esters (CMP2, CMP3, CMP3).

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 2-methoxyethanol; ethylene glycol monomethyl ether | 109-86-4 | Solvent | | 1,000-10,000 | Org | 2 |




**Applications/Markets**

2-Methoxyethanol is used as a solvent for many different purposes such as varnishes, dyes, and resins. It is also used as an additive in airplane de-icing solutions.[2,8]

**Biobased options/(potential) Suppliers/Stakeholders**

Methyl and Ethyl Cellosolve could be replaced by partially alkylated biobased di/triols, like trimethyl glycerol, tertiary butyl glycerol, monomethylisosorbide, etc. One of the few currently commercially available biobased alternatives are lactic acid esters (CMP2, CMP3, CMP3).

## *Organo mercury; entry 20 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 20 | Organo mercury | 2 | - |

No possibilities for biobased.

## *Non-approved PPP; entry 21 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 21 | Non-approved PPP | 2 | 1 |

No possibilities for biobased due to very specific property requirements.

## *Phenols; entry 22 (>100 ton/annum)*

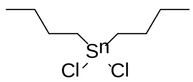
| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 22 | Phenols | 1 | 1 |

No possibilities for biobased due to very specific property requirements.

## *Organotin; entry 24 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 24 | Organotin | 1 | 1 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| dibutyltin dichloride; DBTC | 683-18-1 | Mineral | | 1,000-10,000 | Inorg | 2 |




**Applications/Markets**

As the raw material for the manufacture of other organotin compounds, Dibutyltin Dichloride is invaluable as an intermediate for the manufacture of butyltin based catalysts and PVC stabilizers.

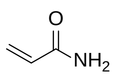
**Biobased options/(potential) Suppliers/Stakeholders**

In case of PVC stabilisers, biobased (co-)stabilisers could be used/developed as alternatives to tin based stabilisers. Stakeholders are e.g. CMP14, CMP15, CMP16, CMP17, CMP18, CMP19.[7]

## *Acrylamide; entry 25 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 25 | Acrylamide | 1 | 1 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Acrylamide | 79-06-1 | Intermediate | | 100,000-1,000,000 | Org | 3 |



**Applications/Markets**

Acrylamide is prepared on an industrial scale by the hydrolysis of acrylonitrile by nitrile hydratase.
Most acrylamide is used to synthesize polyacrylamides (PAM), which find many uses as water-soluble thickeners. These include use in wastewater treatment, papermaking, ore processing, tertiary oil recovery, soil conditioner and the manufacture of permanent press fabrics. Some acrylamide is used in the manufacture of dyes and the manufacture of other monomers.

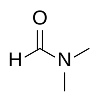
**Biobased options/(potential) Suppliers/Stakeholders**

Biobased, non-acrylate water soluble thickeners. Some types are already available, various are under development (CMP10, CMP11, CMP12, CMP3). Successful implementation will depend on price and technical performance.

## *N,N-dimethylformamide; entry 26 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 26 | N,N-dimethylformamide | 1 | 1 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| N,N-dimethylformamide (DMF) | 68-12-2 | Solvent | | 10,000-100,000 | Org | 2 |




**Applications/Markets**

The primary use of dimethylformamide is as a solvent with low evaporation rate. DMF is used in the production of acrylic fibers and plastics. It is also used in the manufacture of adhesives, synthetic leathers, fibers, films, and surface coatings.

**Biobased options/(potential) Suppliers/Stakeholders**

There is a broadly recognised need for alternatives to polar aprotic solvents, like DMAc, DMF, and NMP. Significant efforts are being undertaken to develop effective, safe biobased alternatives. None are currently commercially available on large scale. Furthermore, no "one-size fits all" solutions have been found yet.

# 4 Conclusions & Shortlist

A quick scan of a selection of the ZZS shows that there is significant potential in biobased replacement of part of the 371 substances considered. As expected, currently many inorganic substances cannot be replaced by biobased alternatives due to their specific physico/chemical properties or requirements; e.g. the use of arsenic in photovoltaic cells or the use of lead oxide in glass manufacturing. Long term developments like e.g. organic solar cells could however open up possibilities in the future.

Some categories are very complex, requiring more time and effort to analyse; such as the petroleum products, but also the coal tar products. Since these categories deal with very large volumes, changes in particular components of integrated chains have impact on the total chain, and hence should be treated with care.

Whereas for some ZZS substances biobased alternatives (level 2 replacement) are already available or in advanced stages of development (e.g. glyme or diglyme alternatives), safe, biobased alternatives for high polarity aprotic solvents such as DMF, DMAc or NMP are still in early development, despite a growing need for replacement. Nevertheless, also here biobased alternatives are possible, yet on longer term (5-10 years). Given the industrial and environmental importance of these solvents, the development of alternatives should be treated with high priority, e.g. by government initiated R&D programmes. For example, a ban on the use of NMP as a dispersing agent could be detrimental to the further development/implementation of (biobased) high solids coatings that serve to reduce VOC emissions.

Also level 3 replacement appears feasible. An example of possible short term implementation is the partial replacement of ethylene oxide for the production of ethylene glycol by the hydrogenolysis of glucose to ethylene glycol and propylene glycol. Other level 3 replacements require more time, and deeper analysis in order to assess the impact on product/value chains.

Overall, this quick scan results in a number of recommendations

- A dedicated follow-up study into the biobased replacement potential for the petroleum products and coal tar products categories.
- Investigate the possibilities for a program on alternative, preferentially biobased, high polarity solvents that can involve the whole value chain, from production to specific applications.
- Specific follow-up studies on ZZS substances for which advanced level replacements have been identified (mid to long term replacements)
- Start a discussion between end-users of the substances on the shortlist, and (potential) producers of biobased alternatives, in order to evaluate the practical feasibility of biobased substitution.

The following table contains a shortlist of nine substances of high concern, for which short-term biobased alternatives have been identified. These alternatives are either already commercially available or close to commercialisation. Hence, the table includes a list of known (potential) suppliers and stakeholders that can be contacted by the RIVM and the ministry for further information. The regulatory status of the substances of very high concern on this shortlist is given in appendix 2.

Biobased replacement shortlist

| Substance | CAS# | Type | Tonnage | BR-Level | (potential) Alternatives | CAS# | (potential) Suppliers |
|---|---|---|---|---|---|---|---|
| bis(2-methoxyethyl) ether, diglyme | 111-96-6 | Solvent | 100-1,000 | 2 | Dimethylisosorbide | 5306-85-4 | CMP1 |
| | | | | | GVL, gamma-valerolactone | 108-29-2 | CMP4 |
| | | | | | ML, methyl levulinate | 624-45-3 | CMP4 |
| | | | | | Lactic acid esters, e.g. ethyl lactate | 97-64-3 | CMP2, CMP3 |
| Stakeholders[A] | CMP8, CMP5, CMP24 (Glymes producers). Glymes are too widely used to pinpoint specific areas of application or specific user groups. Glymes are amongst other used in electrolytes for (lithium batteries), inkjet cartridges, brake fluid, paints and carpet cleaners and active pharmaceutical intermediates (APIs). They are also widely used in the production of printed circuit boards and microchips. Furthermore, glymes are good solvents for oligo- and polysaccharides.[8] | | | | | | |
| 1,2-dimethoxyethane; ethylene glycol dimethyl ether; glyme (EGDME) | 110-71-4 | Solvent | 100-1,000 | 2 | Dimethylisosorbide | 5306-85-4 | CMP1 |
| | | | | | GVL, gamma-valerolactone | 108-29-2 | CMP4 |

[A] *Patent search gives 96 hits on glymes from 2000-2014, yet none related to alternatives.*

| Substance | CAS# | Type | Tonnage | BR-Level | (potential) Alternatives | CAS# | (potential) Suppliers |
|---|---|---|---|---|---|---|---|
| | | | | | ML, methyl levulinate | 624-45-3 | CMP4 |
| | | | | | Lactic acid esters, e.g. ethyl lactate | 97-64-3 | CMP2, CMP3 |
| Stakeholders[A] | CMP8, CMP5, CMP24. Glymes are too widely used to pinpoint specific areas of application or specific user groups. Glymes are amongst other used in electrolytes for (lithium batteries), inkjet cartridges, brake fluid, paints and carpet cleaners and active pharmaceutical intermediates (APIs). They are also widely used in the production of printed circuit boards and microchips. Furthermore, glymes are good solvents for oligo- and polysaccharides.[2,9] | | | | | | |
| 2-nitropropane | 79-46-9 | Intermediate, Solvent | 1,000-10,000 | 2 | Lactic acid esters, e.g. ethyllactate | 97-64-3 | CMP2, CMP3, CMP3 |
| | | | | | ML, methyl levulinate | 624-45-3 | CMP4 |
| Stakeholders[B] | CMP24 was found as a producer. The main application as solvent is in coatings (not specified further).[2,9] The majority of 2-nitropropane is used internally as a chemical intermediate. The remaining product is sold for use primarily as a taggant in the production of C-4 explosives. A very small amount is used for research and development. The role of chemical intermediate cannot be substituted by biobased alternatives. | | | | | | |
| Cyclododecatriene (CDT)[C] | 4904-61-4 | Intermediate | Conf. | 3 | TP1; PA 1010 (= polymer, will fall under REACH polymer exemption ) | | CMP6 |
| | | | | | Castor oil based C10 diacid, sebacic acid | 111-20-6 | CMP9 |
| | | | | | Fatty acid diacids; octadecanedioic acid | 71-70-5 | CMP1, CMP8 |
| Stakeholders | CMP6 (Main CDT producer). Applications are very diverse and include the automotive and wire & cable sectors.[2] No specific markets or | | | | | | |

[A] *Patent search gives 96 hits on glymes from 2000-2014, yet none related to alternatives.*
[B] *Patent search gives 59 hits on nitro and propane from 2000-2014, yet none related to alternatives to 2-nitro-propane.*
[C] *Patent search gives 51 hits on CDT from 2000-2014, all are related to production or purification.*

| Substance | CAS# | Type | Tonnage | BR-Level | (potential) Alternatives | CAS# | (potential) Suppliers |
|---|---|---|---|---|---|---|---|
| | applications are given. | | | | | | |
| Alkanes, C10-13, chloro (Short Chain Chlorinated Paraffins) | 85535-84-8 | Additive | 1,000-10,000 | 2 | Isosorbide esters TP3 | REACH registration pending | CMP21 |
| | | | | | TP2, Fully acetylated glycerol monoester of 12-hydroxystearic acid | 736150-63-3 | CMP22 |
| | | | | | Citrate esters; e.g. Acetyl Tributyl Citrate（ATBC） | 77-90-7 | CMP23 |
| Stakeholders[A] | In 2009, chlorinated paraffins were produced by 78 manufacturers worldwide, including 2 in the United States, 40 in China, and 22 in India [5,6] Chlorinated paraffins are used as extreme-pressure-lubricant additives in metalworking fluids; as flame retardants in plastics, rubber, and paints; to improve water resistance of paints and fabrics; and as a secondary plasticizer in polyvinyl chloride. The suggested alternatives are only feasible in the role of plasticisers for PVC. | | | | | | |
| Propylene oxide | 75-56-9 | Intermediate | 1,000,000 + | 3 | Propylene glycol | 57-55-6 | CMP25, CMP3, CMP24 |
| Stakeholders[B] | CMP28, CMP29, CMP26, CMP24, CMP8 (PO and PG producers).[10] Between 60 and 70% of all propylene oxide is converted to polyether polyols for the production of polyurethane plastics. [less efficient from propylene glycol] About 20% of propylene oxide is hydrolyzed into propylene glycol [2]; 45% of propylene glycol produced is used as chemical feedstock for the production of unsaturated polyester resins (UPR).[11] UPR have a wide variety of applications (usually glass fibre reinforced). The major industries for UPR are Building & Constructions, Automotive/Transportation, Pipes & Tanks, Marine, Wind energy, and Electrical & Electronics. Major players in European and North American regions include CMP30, CMP31, CMP13, CMP32, and CMP33. Like ethylene glycol, propylene glycol is able to lower the freezing point of water, and so it is used as aircraft de-icing fluid. | | | | | | |
| Ethylene oxide | 75-21-8 | Intermediate | 1,000,000 + | 3 | Ethylene glycol directly | 107-21-1 | CMP25, CMP3 |

[A] *No relevant patent found.*
[B] *Subject too broad for efficient patent search.*

| Substance | CAS# | Type | Tonnage | BR-Level | (potential) Alternatives | CAS# | (potential) Suppliers |
|---|---|---|---|---|---|---|---|
| | | | | | from sugars | | |
| Stakeholders[B] | CMP28, CMP5, CMP24, CMP34, CMP8, CMP35, CMP36, CMP26 (EG Producers).[12] EG is primarily used as a raw material in the manufacture of polyester fibers and fabric industry, and polyethylene terephthalate resins (PET) used in bottling, packaging.[2] CMP37, CMP38, CMP39, CMP40, CMP41, CMP42, CMP43 (European PET producers).[13] | | | | | | |
| 2-ethoxyethanol; ethylene glycol monoethyl ether | 110-80-5 | Solvent | 1,000- 10,000 | 2 | Lactic acid esters, e.g. ethyl lactate | 97-64-3 | CMP2, CMP3 |
| | | | | | ML, methyl levulinate | 624-45-3 | CMP4 |
| Stakeholders[A] | A large proportion of glycol ethers go into the paints and coatings industry. Other uses include inks, cleaning products, pharmaceuticals, chemical intermediates, hydraulic and brake fluids, plasticizers, anti-icing agents and cosmetic/personal care products. The use of glycol ethers as solvents in various formulations, such as paints, inks and cleaning fluids accounts for over half of all glycol ether consumption.[8] Specific producers or users of 2-ethoxyethanol are not mentioned. The growth of water-based coatings that use glycol ethers as coalescing agents has been the major factor behind the growth of the entire glycol ether market.[14] The growth in propylene glycol (P-series) glycol ethers has been due primarily to increased concern about the toxicological effects of some ethylene oxide–based glycol ethers. Methyl- and ethyl ethylene glycols are in decline. It is to be expected that these substances will be replaced by other, non-toxic glycol ethers. According to CMP24 ethylene glycol monopropyl ether is useful in printing and other specialized coatings applications. | | | | | | |
| 2-methoxyethanol; ethylene glycol monomethyl ether | 109-86-4 | Solvent | 1,000- 10,000 | 2 | Lactic acid esters, e.g. ethyl lactate | 97-64-3 | CMP2, CMP3 |
| | | | | | ML, methyl levulinate | 624-45-3 | CMP4 |
| Stakeholders[A] | See 2-ethoxyethanol | | | | | | |

[A] *Patent search gives 96 hits on glymes from 2000-2014, yet none related to alternatives.*

**References**

[1] Biobased alternatieven voor prioritaire stoffen : Een verkennende studie. Van Helmond *et al.* 2013: http://www.rivm.nl/Documenten_en_publicaties/Wetenschappelijk/Rapporten/2013/februari/Biobased_alternatieven_voor_prioritaire_stoffen_Een_verkennende_studie.

[2] Source: Wikipedia

[3] Source: ESPA (European Stabiliser Producers Association)

[4] Source: www.petrochemistry.eu; Coal Chemicals Sector Group (CCSG)

[5]Source: http://www.doverchem.com.

[6] Source: http://ntp.niehs.nih.gov/go/roc12.

[7] Source: http://www.stabilisers.org.

[8] Source: http://www.glycol-ethers.eu

[9] Source: EPA

[10] Source: http://www.propylene-glycol.com

[11] Source: http://www.marketsandmarkets.com/PressReleases/unsaturated-polyester-resin-upr.asp; www.cefic.org.

[12] Source: www.petrochemistry.eu.

[13] Source: http://www.cpme-pet.org/members.

[14] Source: http://www.ihs.com/products/chemical/planning/ceh/glycol-ethers.aspx?pu=1&rd=chemihs.

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**Appendix 1**

Overview of EU Regulatory measures in REACH and CLP applicable to the substances included in the shortlist.

| *Substance* | *CAS Number* | *Inclusion in REACH (Regulation EC 1907/2006) Annex XIV (authorisation)* | *Inclusion in REACH (Regulation EC 1907/2006) Annex XVII (restriction)* | *Inclusion in CLP (Regulation EC 1272/2008) Annex VI (harmonised classification)* | *Remarks* |
|---|---|---|---|---|---|
| **bis(2-methoxyethyl) ether, diglyme** | 111-96-6 | Authorisation applies per 22-08-2017; Latest application date: 22-02-2016 | Restriction on the placing on the market and use for supply to the general public (substance, mixture) | Repro Cat 1B | |
| **1,2-dimethoxyethane; ethylene glycol dimethyl ether; glyme (EGDME)** | 110-71-4 | Not included (on candidate list based on SVHC) | Restriction on the placing on the market and use for supply to the general public (substance, mixture) | Repro Cat 1B | |
| **2-nitropropane** | 79-46-9 | Not included | Restriction on the placing on the market and use for supply to the general public (substance, mixture) | Carc. Cat 1B | |
| **Cyclododecatriene (CDT)** | 4904-61-4 | Not included | Not included | Not included | REACH registrations for intermediate and non-intermediate uses |
| **Alkanes, C10-13, chloro (Short Chain Chlorinated Paraffins)** | 855-35-84-8 | Not included (on candidate list based on SVHC) (PBT) | | Not included | |

| | | | | | |
|---|---|---|---|---|---|
| **Propylene oxide** | 75-56-9 | Not included (on candidate list based on SVHC) | Restriction on the placing on the market and use for supply to the general public (substance, mixture) | Carc. Cat 1B<br>Muta. Cat 1B | |
| **Ethylene oxide** | 75-21-8 | Not included | Restriction on the placing on the market and use for supply to the general public (substance, mixture) | Carc. Cat 1B<br>Muta. Cat 1B | |
| **2-ethoxyethanol; ethylene glycol monoethyl ether** | 110-80-5 | Not included (on candidate list based on SVHC) | Restriction on the placing on the market and use for supply to the general public (substance, mixture) | Repro Cat 1B | |
| **2-methoxyethanol; ethylene glycol monomethyl ether** | 109-86-4 | Not included (on candidate list based on SVHC) | Restriction on the placing on the market and use for supply to the general public (substance, mixture) | Repro Cat 1B | |

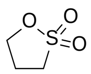
**Appendix 2**

Remaining list of ZZS list substances. BR-Level 0 substances, limited to >100 ton/annum use.

## *Other; entry 2 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 2 | Other | 33 | 15 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 1,3-propanesultone; 1,2-oxathiolane 2,2-dioxide | 1120-71-4 | Intermediate | | 100-1,000 | Org | 0 |



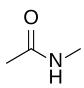

**Applications/Markets**

1,3-Propane sultone is a reactive intermediate for the mild and defined incorporation of sulfonate-groups into organic molecules. The resulting propane sulfonates serves as additives in organic baths, as monomers, colours and wetting agents.

**Biobased options/(potential) Suppliers/Stakeholders**

None; outdated, phased out substance.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| N-methylacetamide | 79-16-3 | Intermediate | | Conf. | Org | 0 |




**Applications/Markets**

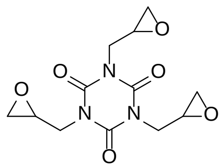
 

Chemical intermediate

**Biobased options/(potential) Suppliers/Stakeholders**

None identified. Difficult to assess replacement options.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione; Triglycidyl isocyanurate (TGIC) | 2451-62-9 | Intermediate | | 100-1,000 | Org | 0 |



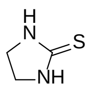
**Applications/Markets**

The main use of triglycidyl isocyanurate is as a three-dimensional cross-linking or curing agent in polyester powder coatings (paints).

**Biobased options/(potential) Suppliers/Stakeholders**

The high reactivity of TGIC is the reason for its toxicity, yet it also makes it very convenient for application in environmentally friendly powder coating resins that make products more durable and reduce the emissions of coating related VOC's. Replacement by biobased epoxides is possible, but will not significantly alter the toxicity due to the inherent reactivity of low molecular weight epoxides.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| ethylene thiourea; imidazolidine-2-thione; 2-imidazoline-2-thiol | 96-45-7 | Intermediate | | 100-1,000 | Org | 0 |



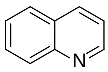
**Applications/Markets**

Ethylene thiourea is used primarily as an accelerator for vulcanizing polychloroprene (neoprene) and polyacrylate rubbers.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| quinoline | 91-22-5 | Intermediate | | 100-1,000 | Org | 0 |



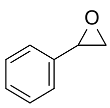
**Applications/Markets**

Quinoline is used in the manufacture of dyes, the preparation of hydroxyquinoline sulfate and niacin. It has also used as a solvent for resins and terpenes. Quinoline is mainly used as a feedstock in the production of other specialty chemicals. Its principal use is as a precursor to 8-hydroxyquinoline, which is a versatile chelating agent and precursor to pesticides. Its 2- and 4-methyl derivatives are precursors to cyanine dyes. Oxidation of quinoline affords quinolinic acid (pyridine-2,3-dicarboxylic acid), a precursor to the herbicide sold under the name "Assert".

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| styrene oxide; (epoxyethyl)benzene; phenyloxirane | 96-09-3 | Intermediate | | 100-1,000 | Org | 0 |



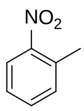
**Applications/Markets**

Styrene oxide is used as a reactive plasticizer or diluent for epoxy resins; in the production of styrene glycol and its derivatives; as a raw material for the production of phenethyl alcohol used in perfumes; as a chemical intermediate for cosmetics, surface coatings, and agricultural and biological chemicals; and in the treatment of fibers and textiles.

**Biobased options/(potential) Suppliers/Stakeholders**

Biobased alternative epoxides will probably have similar toxicological effects as styrene oxide**.**

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 2-nitrotoluene | 88-72-2 | Intermediate | | 10,000-100,000 | Org | 0 |



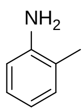

**Applications/Markets**

Chemical intermediate for *o*-toluidine.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| o-toluidine | 95-53-4 | Intermediate | | 10,000-100,000 | Org | 0 |




**Applications/Markets**

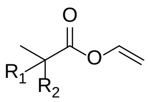
Chemical intermediate for the production of dyes. They are a component of accelerators for cyanoacrylate glues.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Neodecanoic acid vinyl ester | 51000-52-3 | Intermediate | | 10,000-100,000 | Org | 0 |




Vinyl ester of mixture of carboxylic acids with the common structural formula $C_{10}H_{20}O_2$

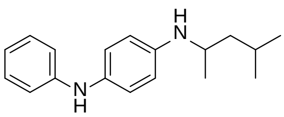
**Applications/Markets**

VeoVa 10 Monomer (Momentive Specialty Chemicals) is widely used as a modifying co-monomer in the manufacture of vinyl acetate based polymer latices. VeoVa 10 Monomer is also used for the production of VeoVa 10/(meth)acrylic latices and solution polymers.

**Biobased options/(potential) Suppliers/Stakeholders**

None. Toxicological effects probably inherently related to vinyl ester functionality.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylene diamine (6PPD) | 793-24-8 | Additive | | 10,000-100,000 | Org | 0 |




**Applications/Markets**

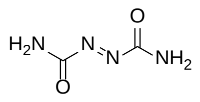
6PPD functions as a powerful antioxidant and antiozonant for natural and synthetic elastomer compounds (e.g. tire components) and as a synthetic polymer stabilizer. Santoflex™ 6PPD (Eastman Chemical) provides protection against fatigue degradation in both static and dynamic operating conditions

**Biobased options/(potential) Suppliers/Stakeholders**

None. Too specific.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Azodicarbonamide | 123-77-3 | Intermediate | | 10,000-100,000 | Org | 0 |



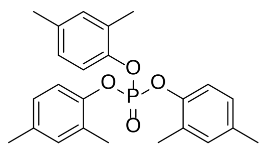

**Applications/Markets**

The principal use of azodicarbonamide is in the production of foamed plastics as a blowing agent. The thermal decomposition of azodicarbonamide results in the evolution of nitrogen, carbon monoxide, carbon dioxide, and ammonia gases, which are trapped in the polymer as bubbles to form a foamed article.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Trixylyl phosphate (TXP) | 25155-23-1 | Additive | | 1,000-10,000 | Org | 0 |




**Applications/Markets**

Hydraulic Fluids; Industrial uses but not in consumer articles .

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical and physical properties to allow for (biobased) substitution.

## *Lead/lead compounds; entry 3 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 3 | Lead/lead compounds | 26 | 26 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Lead (II) oxide (PbO) | 1317-36-8 | Intermediate | | 100,000-1,000,000 | Inorg | 0 |

**Applications/Markets**

Modern applications for PbO are mostly in lead-based industrial glass and industrial ceramics, including computer components. The consumption of lead, and hence the processing of PbO, correlates with the number of automobiles because it remains the key component of automotive lead-acid batteries.[i]

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Lead oxide sulfate | 12036-76-9 | Intermediate | | 100-1,000 | Inorg | 0 |

**Applications/Markets**

A number of lead basic sulfates are known: $PbSO4 \cdot PbO$; $PbSO4 \cdot 2PbO$; $PbSO4 \cdot 3PbO$; $PbSO4 \cdot 4PbO$. They are used in manufacturing of active paste for lead acid batteries.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Lead titanium zirconium oxide, Lead zirconate titanate (PZT) | 12626-81-2 | Intermediate | | 100-1,000 | Inorg | 0 |

**Applications/Markets**

PZT is a ceramic perovskite material that shows a marked piezoelectric effect, which finds practical applications in the area of electroceramics. Being pyroelectric, this material develops a voltage difference across two of its faces when it experiences a temperature change. As a result, it can be used as a heat sensor. PZT is used to make ultrasound transducers and other sensors and actuators, as well as high-value ceramic capacitors and FRAM chips.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Orange lead (lead tetroxide) | 1314-41-6 | Intermediate | | 10,000-100,000 | Inorg | 0 |

**Applications/Markets**

Lead(II,IV) oxide is used in the manufacture of batteries, lead glass and rust-proof primer paints.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Pentalead tetraoxide sulphate | 12065-90-6 | Intermediate | | 100,000-1,000,000 | Inorg | 0 |

**Applications/Markets**

A number of lead basic sulfates are known: $PbSO_4 \cdot PbO$; $PbSO_4 \cdot 2PbO$; $PbSO_4 \cdot 3PbO$; $PbSO_4 \cdot 4PbO$. They are used in manufacturing of active paste for lead acid batteries.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Silicic acid, lead salt | 11120-22-2 | Intermediate | | 100-1,000 | Inorg | 0 |

**Applications/Markets**

Ceramic flux.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Tetraethyllead (TEL) | 78-00-2 | Additive | | 1,000-10,000 | Inorg/Org | 0 |

**Applications/Markets**

TEL is still used as an additive in some grades of aviation gasoline, and in some developing countries.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Tetralead trioxide sulphate (Tribasic Lead Sulphate) | 12202-17-4 | Additive | | 1,000,000-10,000,000 | Inorg | 0 |

**Applications/Markets**

A number of lead basic sulfates are known: $PbSO4 \cdot PbO$; $PbSO4 \cdot 2PbO$; $PbSO4 \cdot 3PbO$; $PbSO4 \cdot 4PbO$. They are used in manufacturing of active paste for lead acid batteries.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

## *Nickel/nickel compounds; entry 4 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 4 | Nickel/nickel compounds | 15 | - |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Nickel Sulfide (NiS) | 79-16-3 | Ore | | 10,000-100,000 | Inorg | 0 |

**Applications/Markets**

Nickel Ore

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Nickel(II) chloride ($NiCl_2$) | 7718-54-9 | Ore | | 10,000-100,000 | Inorg | 0 |

**Applications/Markets**

In general nickel(II) chloride, in various forms, is the most important source of nickel for chemical synthesis. Nickel chloride solutions are used for electroplating nickel onto other metal items.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Nickel(II) hydroxide ($NiOH_2$) | 12054-48-7 | Intermediate | | 1,000-10,000 | Inorg | 0 |

**Applications/Markets**

Due to reactivity in redox processes nickel (II) hydroxide is frequently used in electrochemical cells. In particular, as a good capacitor, it is frequently used for the storage of electrochemical energy. For example, it has been proposed as a useful electrode for use in electrical car batteries.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Nickel(II) dinitrate ($Ni(NO_3)_2$) | 13138-45-9 | Intermediate | | 1,000-10,000 | Inorg | 0 |

**Applications/Markets**

Precursor for industrial nickel hydrogenation catalysts.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Nickel(II) sulphate ($NiSO_4$) | 7786-81-4 | Intermediate | | 10,000-100,000 | Inorg | 0 |

**Applications/Markets**

The salt is usually obtained as a by-product of copper refining. It is also produced by dissolution of nickel metal or nickel oxides in sulfuric acid. It is mainly used for electroplating of nickel.[1]

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| [carbonato(2-)] tetrahydroxytrinickel, basic nickel carbonate | 9863-10-3 | Intermediate | | 1,000-10,000 | Inorg | 0 |

**Applications/Markets**

From the industrial perspective, the most important nickel carbonate **is basic nickel carbonate** with the formula $Ni_4CO_3(OH)_6(H_2O)_4$. The basic carbonate is an intermediate in the hydrometallurgical purification of nickel from its ores and is used in electroplating of nickel. Nickel carbonates are used in some ceramic applications and as precursors to catalysts.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| nickel di(acetate) | 373-02-4 | Intermediate | | 100-1,000 | Inorg | 0 |

**Applications/Markets**

Nickel(II) acetate is used for electroplating.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| dialuminium nickel tetraoxide, Nickel aluminate | 12004-35-2 | Intermediate | | 100-1,000 | Inorg | 0 |

**Applications/Markets**

Component of hydrotreating catalysts.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| nickel bis(sulfamidate); nickel sulfamate | 13770-89-3 | Intermediate | | 100-1,000 | Inorg | 0 |

**Applications/Markets**

Sulfamate nickel plating is used for many engineering applications. It is deposited for dimensional corrections, abrasion and wear resistance, and corrosion protection. It is also used as an undercoat for chromium.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| nickel difluoride | 10028-18-9 | Intermediate | | 100-1,000 | Inorg | 0 |

**Applications/Markets**

Nickel(II) fluoride is the chemical compound with the formula NiF2. Unlike many fluorides, NiF2 is stable in air. NiF2 comprises the passivating surface that forms on nickel alloys, e.g. monel, which is why such materials are good to store or transport hydrogen fluoride or elemental fluorine. Nickel is one of the few materials that can be used to store fluorine because it forms this coating.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| trinickel disulfide; nickel subsulfide | 12035-72-2 | Intermediate | | 100-1,000 | Inorg | 0 |

**Applications/Markets**

Nickel subsulfide is produced in nickel refineries and used in the manufacture of lithium batteries.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| nickel bis(dihydrogen phosphate) | 18718-11-1 | Intermediate | | 100-1,000 | Inorg | 0 |

**Applications/Markets**

None found.

**Biobased options/(potential) Suppliers/Stakeholders**

None.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| nickel bis(2-ethylhexanoate), nickel octaoate | 4454-16-4 | Catalysts | | 100-1,000 | Org/Inorg | 0 |

**Applications/Markets**

Homogeneous catalysts.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

## *Boron/boron compounds; entry 6 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 6 | Boron/boron compounds | 10 | 5 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| diboron trioxide; boric oxide | 1303-86-2 | Intermediate | | 1,000-10,000 | Inorg | 0 |

**Applications/Markets**

Diboron trioxideis a fluxing agent for glass and enamels, a starting material for synthesizing other boron compounds such as boron carbide. It is also used in the production of borosilicate glass

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| perboric acid sodium salt | 11138-47-9 | Additive | | 10,000-100,000 | Inorg | 0 |
| perboric acid, sodium salt, monohydrate | 12040-72-1 | Additive | | 10,000-100,000 | Inorg | 0 |
| perboric acid, sodium salt, tetrahydrate | 37244-98-7 | Additive | | 10,000-100,000 | Inorg | 0 |

**Applications/Markets**

It serves as a source of active oxygen in many detergents, laundry detergents, cleaning products, and laundry bleaches. It has antiseptic properties and can act as a disinfectant.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| boric acid | 10043-35-3 | | | 100,000-1,000,000 | Inorg | 0 |

**Applications/Markets**

The primary industrial use of boric acid is in the manufacture of monofilament fiberglass usually referred to as textile fiberglass. Textile fiberglass is used to reinforce plastics in applications that range from boats, to industrial piping to computer circuit boards. Boric acid is used in the production of the glass in LCD flat panel displays. Boric acid, mixed with borax (sodium tetraborate decahydrate) at the weight ratio of 4:5, is highly soluble in water, though they are not so soluble separately. The solution is used for fire retarding agent of wood by impregnation. Boric acid, in combination with silicone oil, is used to manufacture Silly Putty. Boric acid, in combination with eighty other chemicals, is used in Marcellus Shale hydraulic fracturing.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| disodium tetraborate, anhydrous | 1330-43-4 | Mineral | | 100,000-1,000,000 | Inorg | 0 |
| disodium tetraborate decahydrate | 1303-96-4 | Mineral | | 100,000-1,000,000 | Inorg | 0 |
| borax decahydrate | 1330-43-4 | Mineral | | 100,000-1,000,000 | Inorg | 0 |
| disodium tetraborate pentahydrate | 12179-04-3 | Mineral | | 100,000-1,000,000 | Inorg | 0 |

Borax: The term borax is often used for a number of closely related minerals or chemical compounds that differ in their crystal water content.

**Applications/Markets**

Borax is used in various household laundry and cleaning products. It is a precursor for sodium perborate monohydrate that is used in detergents, as well as for boric acid and other borates. Ingredient in enamel glazes. Component of glass, pottery, and ceramics. Fire retardant

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

## *Cadmium/cadmium compounds; entry 7 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 7 | Cadmium/cadmium compounds | 6 | 4 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| cadmium oxide (non-pyrophoric) | 1306-19-0 | Mineral | | 1,000 - 10,000 | Inorg | 0 |
| cadmium (non-pyrophoric) | 7440-43-9 | Mineral | | 1,000 - 10,000 | Inorg | 0 |
| cadmium (pyrophoric) | 7440-43-9 | Mineral | | 1,000 - 10,000 | Inorg | 0 |
| Cadmium and cadmium | 7440-43-9 | Mineral | | 1,000 - 10,000 | Inorg | 0 |

| |
|---|
| compounds |

**Applications/Markets**

Cadmium occurs as a minor component in most zinc ores and therefore is a byproduct of zinc production. Cadmium oxide is one of the main precursors to other cadmium compounds. Cadmium oxide is used in cadmium plating baths, electrodes for storage batteries, cadmium salts, catalyst, ceramic glazes, phosphors, and nematocide. Major uses for cadmium oxide are as an ingredient for electroplating baths, and in pigments.
One of its few new uses is in cadmium telluride solar panels. Cadmium electroplating, consuming 6% of the global production, can be found in the aircraft industry due to the ability to resist corrosion when applied to steel components. This coating is passivated by the usage of chromate salts. In paint pigments, cadmium forms various salts, with CdS being the most common. This sulfide is used as a yellow pigment.

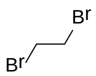
**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

## *Br/Cl hydrocarbons; entry 8 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 8 | Br/Cl hydrocarbons | 7 | 3 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 1,2-dibromoethane (EDB) | 106-93-4 | Pesticide | | 1,000-10,000 | Org | 0 |




**Applications/Markets**

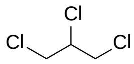
EDB continues to be used as a fumigant for treatment of logs for termites and beetles, for control of moths in beehives.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 1,2,3-Trichloropropane (TCP) | 96-18-4 | Intermediate | | 1,000-10,000 | Org | 0 |



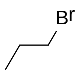

**Applications/Markets**

1,2,3-TCP had been used in the past primarily as a solvent for paint and varnish removal, as a cleaning and degreasing agent, and as a cleaning and maintenance solvent. No current information is available to indicate that it continues to be used for these purposes. 1,2,3-TCP is currently used as an intermediate in the production of polysulfone liquid polymers, the synthesis of hexafluoropropylene, and as a cross-linking agent in the synthesis of polysulfides. Polysulfone liquid polymers are used in the following industries: aerospace, automotive,consumer goods, electrical and electronic, health care, and in industrial equipment, such as compressor and pump valve components. Hexafluoropropylene is a fluorointermediate that is a key building block required to produce Teflon fluoropolymers. Polysulfides are used as catalyst sulfidation agents and in the formulation of lubricant additives created for use in high-pressure environments or applications.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 1-bromopropane; n-propyl bromide (NPB) | 106-94-5 | Solvent | | 1,000-10,000 | Org | 0 |




**Applications/Markets**

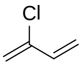
Like other halocarbons, n-propyl bromide finds use as a solvent. It is used for the cleaning of metal surfaces, removal of soldering residues from electronic circuit boards. It is also a solvent for adhesives. It has been deployed as a replacement for perchloroethylene as a dry cleaning solvent. It is also used in the hole transport layer (HTL) of multi-layered OLEDs. The chemical's increasing use in the 21st century resulted from need for a substitute for chlorofluorocarbons and perchloroethylene (tetrachloroethylene). It has been approved for use under the U.S. EPA's Significant New Alternatives Policy (SNAP) as a suitable replacement for ozone depleting chemicals.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Chloroprene, 2-chlorobuta-1,3-diene | 126-99-8 | | | 10,000-100,000 | Org | 0 |



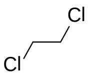

**Applications/Markets**

This colorless liquid is the monomer for the production of the polymer polychloroprene, a type of synthetic rubber. Polychloroprene is better known to the public as Neoprene, the trade name given by DuPont.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 1,2-dichloroethane; ethylene dichloride (EDC) | 107-06-2 | Intermediate | | 1,000,000-10,000,000 | Org | 0 |




**Applications/Markets**

Ethylene dichloride (EDC), is a chlorinated hydrocarbon, mainly used to produce vinyl chloride monomer (VCM, chloroethene), the major precursor for PVC production. As a useful 'building block' reagent, it is used as an intermediate in the production of various organic compounds such as ethylenediamine.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.
Although one could envision level 3 replacement by replacing PVC by biobased polymers, this option is highly challenging due to various specific advantages of PVC over other polymers, and the fact that EDC is one of the main outlets for chorine, which is produced during the production of the base chemical sodium hydroxide by electrolysis of brine.

## *Chromium/chromium compounds; entry 10 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 10 | Chromium/chromium compounds | 4 | 4 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| strontium chromate | 7789-06-2 | Additive | | 1,000 - 10,000 | Inorg | 0 |

**Applications/Markets**

Corrosion inhibitor in pigments, as colorant in polyvinyl chloride resins, and as an anti-corrosive primer for zinc, magnesium, aluminum, and alloys used in aircraft manufacture.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Potassium hydroxyoctaoxodizincatedichromate | 11103-86-9 | Additive | | 100 - 1000 | Inorg | 0 |

**Applications/Markets**

Used in industrial sealants and coatings in the aerospace sector and vehicle sector (fleet and commercial vehicles, heavy duty vehicles and trucks, military vehicles and agricultural equipment).

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

## *Cobalt/cobalt compounds; entry 11 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 11 | Cobalt/cobalt compounds | 4 | 4 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Cobalt(II) dinitrate | 10141-05-6 | Intermediate | | 1,000 - 10,000 | Inorg | 0 |

**Applications/Markets**

It is commonly reduced to metallic cobalt or precipitated on various substrates for Fischer-Tropsch catalysis.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Cobalt(II) sulphate | 10124-43-3 | Intermediate | | 1,000 - 10,000 | Inorg | 0 |

**Applications/Markets**

Cobalt(II) sulfate is used in the preparation of pigments, as well as in the manufacture of other cobalt salts. Cobalt pigment is used in porcelains and glass. Cobalt(II) sulfate is used in storage batteries and electroplating baths, sympathetic inks, and as an additive to soils and animal feeds.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Cobalt(II) carbonate | 513-79-1 | | | 1,000 - 10,000 | Inorg | 0 |

**Applications/Markets**

Cobalt carbonate is a precursor to cobalt carbonyl and various cobalt salts. It is a component of dietary supplements since cobalt is an essential element. It is a precursor to blue pottery glazes, famously in the case of Delftware.

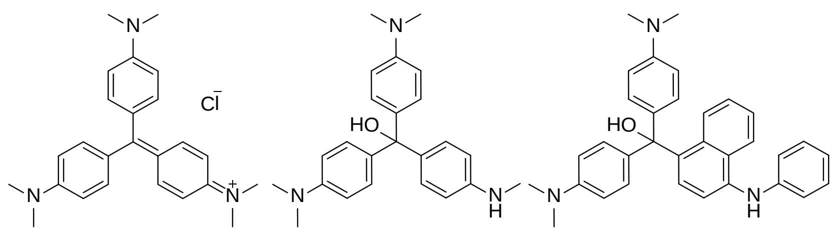
**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

### *Azo dyes; entry 13 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 13 | Azo dyes | 3 | 3 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| C.I. Basic Violet 3, Crystal violet or gentian violet | 548-62-9 | Additive | | 1-10 | Org | 0 |
| 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol | 561-41-1 | Additive | | 1-10 | Org | 0 |
| α,α-Bis[4-(dimethylamino)phenyl]-4 (phenylamino)naphthalene-1-methanol (C.I. Solvent Blue 4) | 6786-83-0 | Additive | | 10-100 t | Org | 0 |



All below 100 ton

Too specific.

### *Hydrazines; entry 14 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 14 | Hydrazines | 3 | 2 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Hydrazine | 302-01-2 | Intermediate | | 10,000- | Inorg | 0 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| | | | | 100,000 | | |
| hydrate(s) of hydrazine | 7803-57-8 | Intermediate | | 10,000-100,000 | Inorg | 0 |

$H_2N-NH_2$

**Applications/Markets**

Hydrazine is mainly used as a foaming agent in preparing polymer foams, but significant applications also include its uses as a precursor to polymerization catalysts and pharmaceuticals. Additionally, hydrazine is used in various rocket fuels and to prepare the gas precursors used in air bags. Hydrazine is used within both nuclear and conventional electrical power plant steam cycles as an oxygen scavenger to control concentrations of dissolved oxygen in an effort to reduce corrosion. The majority use of hydrazine is as a precursor to blowing agents. Specific compounds include azodicarbonamide and azobisisobutyronitrile, which yield 100-200 mL of gas per gram of precursor. In a related application, sodium azide, the gas-forming agent in air bags, is produced from hydrazine by reaction with sodium nitrite.

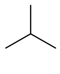
**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

## *Butadiene(s); entry 15 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 15 | Butadiene(s) | 3 | - |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| isobutane | 75-28-5 | Propellant | | 1,000,000-10,000,000 | Org | 0 |

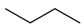


**Applications/Markets**

Isobutane is used as a refrigerant. Isobutane is also used as a propellant for aerosol cans and foam products.
**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific physical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| n-butane | 106-97-8 | Intermediate | | 1,000,000-10,000,000 | Org | 0 |



**Applications/Markets**

Normal butane is mainly used for gasoline blending, as a fuel gas, either alone or in a mixture with propane, and as a feedstock for the manufacture of ethylene and butadiene.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific physical and chemical properties to allow for (biobased) substitution.

## *Beryllium; entry 16 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 16 | Beryllium | 2 | - |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| beryllium oxide | 1304-56-9 | Mineral | | 1-10 | Inorg | 0 |
| beryllium | 7440-41-7 | Mineral | | 10- 100 | Inorg | 0 |

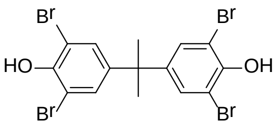
All below 1000 tons

## *Brominated flame retardants; entry 17 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 17 | Brominated flame retard. | 2 | 1 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Tetrabromobisphenol A; TBBP-A | 79-94-7 | Additive | | 1,000-10,000 | Org | 0 |



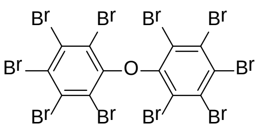

**Applications/Markets**

TBBPA can be used as reactive and additive flame retardant. In the reactive application, TBBPA is bound chemically to the polymers. The main use are epoxy resins of printed circuit boards. As an additive flame retardant it is used in acrylonitrile butadiene styrene, which are used e.g. in TVs.

**Biobased options/(potential) Suppliers/Stakeholders**

Too specific: brominated flame retardants are highly efficient, and work synergistically with $Sb_2O_3$. Brominated biobased substances can be developed, yet these can have the same detrimental toxicological effects.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Decabromodiphenyl ether; DecaBDE | 1163-19-5 | Additive | | 10,000-100,000 | Org | 0 |




**Applications/Markets**

DecaBDE is a flame retardant. The chemical "is always used in conjunction with antimony trioxide" in polymers, mainly in "high impact polystyrene (HIPS) which is used in the television industry for cabinet backs." DecaBDE is also used for "polypropylene drapery and upholstery fabric" by means of backcoating and "may also be used in some synthetic carpets."

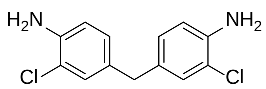
**Biobased options/(potential) Suppliers/Stakeholders**

Too specific: brominated flame retardants are highly efficient, and work synergistically with $Sb_2O_3$. Brominated biobased substances can be developed, yet these can have the same detrimental toxicological effects.

## *Chlorinated aromatics; entry 18 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 18 | Chlorinated aromatics | 2 | 1 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| 2,2'-dichloro-4,4'-methylenedianiline; 4,4'-methylene bis(2-chloroaniline) (MOCA) | 101-14-4 | Intermediate | | 1,000-10,000 | Org | 0 |




**Applications/Markets**

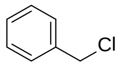
The main use of MOCA is as a curing agent in the manufacture of polyurethane. This use is within the scope of authorisation (ECHA, 2011). MOCA is here not used to manufacture a substance, polyurethane for instance, but to provide specific properties, such as high abrasion resistance, heat, fuel and solvent resistance, high load-bearing and good mechanical and dynamic properties to the already existing substance (ECHA, 2011).

**Biobased options/(potential) Suppliers/Stakeholders**

Too specific.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| α-chlorotoluene; benzyl chloride | 100-44-7 | Intermediate | | 10,000-100,000 | Org | 0 |




**Applications/Markets**

Industrially, benzyl chloride is the precursor to benzyl esters which are used as plasticizer, flavorants, and perfumes. Phenylacetic acid, a precursor to pharmaceuticals, arises via benzyl cyanide, which is generated by treatment of benzyl chloride with sodium cyanide. Quaternary ammonium salts, used as surfactants, are readily formed by alkylation of tertiary amines with benzyl chloride.[1]

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific inherent chemical properties to allow for (biobased) substitution.

## *Organo mercury; entry 20 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 20 | Organo mercury | 2 | - |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| mercury | 7439-97-6 | Mineral | | 100- 1,000 | Inorg | 0 |
| mercury and organic mercury compounds | 7439-97-6 | Mineral | | 100- 1,000 | Inorg | 0 |

Less than 1000 tons

Mercury is used primarily for the manufacture of industrial chemicals or for electrical and electronic applications. It is used in some thermometers, especially ones which are used to measure high temperatures. A still increasing amount is used as gaseous mercury in fluorescent lamps, while most of the other applications are slowly phased out due to health and safety regulations. By far the largest use of mercury in the late 20th century was in the mercury cell process (also called the Castner-Kellner process) where metallic sodium is formed as an amalgam at a cathode made from mercury; this sodium is then reacted with water to produce sodium hydroxide.

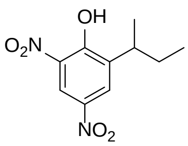
**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific physical properties to allow for (biobased) substitution.

## *Non-approved PPP; entry 21 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 21 | Non-approved PPP | 2 | 1 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| dinoseb | 88-85-7 | Herbicide | | 1000-10,000 | Org | 0 |




**Applications/Markets**

Banned Herbicide

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Carbon monoxide, CO | 630-08-0 | Intermediate | | 100,000-1,000,000 | Org | 0 |

**Applications/Markets**

Carbon monoxide is an industrial gas that has many applications in bulk chemicals manufacturing. Large quantities of aldehydes are produced by the hydroformylation reaction of alkenes, carbon monoxide, and H2. Phosgene, useful for preparing isocyanates, polycarbonates, and polyurethanes, is produced by passing purified carbon monoxide and chlorine gas through a bed of porous activated carbon, which serves as a catalyst. Methanol is produced by the hydrogenation of carbon monoxide. In a related reaction, the hydrogenation of carbon monoxide is coupled to C-C bond formation, as in the Fischer-Tropsch process where carbon monoxide is hydrogenated to liquid hydrocarbon fuels. This technology allows coal or biomass to be converted to diesel. In the Monsanto process, carbon monoxide and methanol react in the presence of a homogeneous rhodium catalyst and hydroiodic acid to give acetic acid. This process is responsible for most of the industrial production of acetic acid.

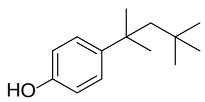
**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

## *Phenols; entry 22 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 22 | Phenols | 1 | 1 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| octylphenol; 4-(1,1,3,3-tetramethylbutyl)phenol; 4-tert-Octylphenol | 140-66-9 | Intermediate | | 10,000-100,000 | Org | 0 |




**Applications/Markets**

Registration dossiers for 4-tert-octylphenol indicate that its ethoxylates are used in formulation of paints, industrial end-use of paints, consumer and professional end-use of paints and other products, in emulsion polymerisation, and as an intermediate in the production of ether sulphates. It seems that almost 50% of the 4-tert-OPnEO is used as emulsifiers in emulsion polymerisation (Annex XV report). In the public consultation industry (CEPAD/APERC) stated that 4-tert- OPnEOs "are used predominantly in the formulation of paint and coating products and are used at levels of generally 1% or less in those products" (RCOM, 2014).

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.

## *Arsenic compounds; entry 23 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 23 | Arsenic compounds | 1 | - |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Gallium arsenide (GaAs) | 140-66-9 | Mineral | | 10- 100 | Inorg | 0 |

**Applications/Markets**

Semiconductors, PV cells, laser diodes, LEDs

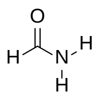
**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical and physical properties to allow for (biobased) substitution.

## *Formamide; entry 27 (>100 ton/annum)*

| Entry | Substance group | # ZZS registered Substances | # on Annex XIV candidate list |
|---|---|---|---|
| 27 | Formamide | 1 | 1 |

| Substance | CAS# | Type | Annex XIV | Tonnage | Org/Inorg | BR-Level |
|---|---|---|---|---|---|---|
| Formamide | 75-12-7 | Solvent | | 10- 100 | Org | 0 |




**Applications/Markets**

It is chemical feedstock for the manufacture of sulfa drugs, other pharmaceuticals, herbicides, pesticides and the manufacture of hydrocyanic acid.

**Biobased options/(potential) Suppliers/Stakeholders**

None, this substance has too specific chemical properties to allow for (biobased) substitution.