OSPAR COMMISSION

Background Document on neodecanoic acid, ethenyl ester

Hazardous Substances Series

2011

OSPAR Convention

The Convention for the Protection of the Marine Environment of the North-East Atlantic (the "OSPAR Convention") was opened for signature at the Ministerial Meeting of the former Oslo and Paris Commissions in Paris on 22 September 1992. The Convention entered into force on 25 March 1998. It has been ratified by Belgium, Denmark, Finland, France, Germany, Iceland, Ireland, Luxembourg, Netherlands, Norway, Portugal, Sweden, Switzerland and the United Kingdom and approved by the European Union and Spain.

Convention OSPAR

La Convention pour la protection du milieu marin de l'Atlantique du Nord-Est, dite Convention OSPAR, a été ouverte à la signature à la réunion ministérielle des anciennes Commissions d'Oslo et de Paris,
à Paris le 22 septembre 1992. La Convention est entrée en vigueur le 25 mars 1998.
La Convention a été ratifiée par l'Allemagne, la Belgique, le Danemark, la Finlande, la France, l'Irlande, l'Islande, le Luxembourg, la Norvège, les Pays-Bas, le Portugal, le Royaume-Uni de Grande Bretagne et d'Irlande du Nord, la Suède et la Suisse et approuvée par l'Union européenne et l'Espagne.

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Executive Summary

Neodecanoic acid, ethenyl ester (CAS No. 51000-51-3), also known as vinyl neodecanoate, is an ester and mixture of isomers mainly used as a synthetic intermediate in the production of polymeric binding agents for use in latex coatings. It may also be used in adhesives and for the production of solvent-borne vinyl neodecanoate-based polymers and powders. There is presently no evidence for the substance being used as such (i.e. unreacted); it is generally used as co-, ter- or higher monomer in polymerisation processes. Vinyl neodecanoate was added to the OSPAR List of Chemicals for Priority Action in 2000.

Vinyl neodecanoate is produced in the EU at one site in the Netherlands that supplies the global market. The amount of the substance sold in the EU and polymerised into latex is estimated to 29 000 tonnes in 2003, but more recent information suggest that quantities are significantly higher.

There is a potential risk for the marine environment from the use of vinyl neodecanoate and the latex polymer products. There is a need to refine the risk evaluation with further information and/or testing. This includes better exposure information to refine PECs and also, if required, further testing on freshwater aquatic and/or marine organsims to reduce the uncertainties over the PNEC. There is no indication about the location of any of the sites polymerising the substance into latex polymers in the EU, but it is quite possible that some are in coastal regions. Such inforamtion should be sought, together with inforamtion on marine releases, and used to refine the marine assessment.A proper evaluation of the appropriate choices for action, including risk reduction scenarios, can only be made if necessary after the risk assessment has been further refined. The actions recommended are: to ensure that the information in this background document and the conclusions reached by OSPAR are generally taken into account in the approach of the European Union; to invite relevant industries to work with Contracting parties to provide further information on the substance's persistence and to improve the estimates of emissions, and if necessary, the estimation of PNEC values so that the moste effective risk reduction measures can be adopted if required; to re-evaluate the risk posed by vinyl neodecanoate when further information has been collected; to ensure that information in this background document can be considered in the context of other international agreements which deal with hazardous substances.

Récapitulatif

L'ester éthylique d'acide néodécanoïque (CAS No. 51000-51-3), également appelé néodécanoate de vinyle, est un ester et un mélange d'isomères utilisé principalement en tant que produit synthétique intermédiaire dans la production des agents liants polymériques utilisés dans les revêtements en latex. On peut également l'utiliser dans les adhésifs et dans la production de polymères et poudres à base de néodécanoate de vinyle en phase solvant. Il ne semble pas à l'heure actuelle que cette substance soit utilisée de cette manière (c'est-à-dire non polymérisée); elle est généralement utilisée en tant que co-, ter- ou plus monomère au cours de processus de polymérisation. Le néodécanoate de vinyle a été ajouté à la Liste OSPAR des produits chimiques prioritaires en 2000.

Le néodécanoate de vinyle est produit dans l'Union européenne (UE) dans un site aux Pays-Bas qui fournit le marché mondial. On estime que les quantités de cette substance, vendues au sein de l'UE et polymérisée en latex, en 2003 s'élèvent 29 000 tonnes, mais des informations plus récentes suggèrent que ces quantités sont beaucoup plus élevées.

L'utilisation du néodécanoate de vinyle et des polymères du latex présente un risque potentiel pour le milieu marin. Il y a lieu d'affiner l'évaluation du risque grâce à des informations et/ou des vérifications supplémentaires. Il s'agit notamment d'obtenir de meilleures informations sur l'exposition pour affiner les PNEC et également, si besoin est, d'effectuer des vérifications supplémentaires sur les organismes aquatiques d'eau douce et/ou marins afin de réduire les incertitudes des PNEC. On ne possède aucune

information sur l'emplacement d'un quelconque site de polymérisation de cette substance en latex dans l'UE, mais il est fort possible que certains soient situés dans les régions côtières. Il faudra obtenir ces informations ainsi que celles sur les rejets marins et les utiliser pour affiner les évaluations marines.

On ne peut réaliser, si besoin est, une évaluation véritable des mesures appropriées à sélectionner, notamment les scénarios de réduction du risque, qu'après avoir affiné plus avant l'évaluation du risque. Les mesures recommandées sont les suivantes: s'assurer que les informations figurant dans le présent document de fond ainsi que les conclusions d'OSPAR sont généralement prises en compte dans l'approche adoptée par l'UE; inviter les industries pertinentes à travailler avec les Parties contractantes afin d'obtenir des informations supplémentaires sur la persistance de cette substance et améliorer les estimations des émissions et, si besoin est, les estimations des valeurs PNEC pour pouvoir adopter les mesures de réduction du risque les plus efficaces, le cas échéant; évaluer à nouveau le risque que présente le néodécanoate de vinyle une fois que des informations supplémentaires ont été recueillies; s'assurer que les informations figurant dans le présent document de fond peuvent être considérées dans le contexte d'autres accords internationaux s'occupant de substances dangereuses.

1. Basis and rationale for action

The objective stated in the OSPAR Strategy with regard to Hazardous Substances ('the Strategy'), which was adopted in Sintra in 1998, updated at the 2003 and 2010 Ministerial Meetings and endorsed by Ministers is:

> *"to prevent pollution of the maritime area by continuing to reduce discharges, emissions and losses of hazardous substances, with the ultimate aim of achieving concentrations in the marine environment near background values for naturally occurring substances and close to zero for man-made synthetic substances".*

The Strategy also includes a timeframe which states that:

> *"every endeavour will be made to move towards the target of cessation of discharges, emissions and losses of hazardous substances by the year 2020".*

Neodecanoic acid, ethenyl ester is more commonly known as vinyl neodecanoate, and this name is used in this Background Document. Vinyl neodecanoate (CAS 51000-52-3) is on the OSPAR List of Chemicals for Priority Action, and the UK is the lead country for drawing up a background document on the substance.

This Background Document addresses this obligation and has the following aims:

- identifying the main sources of vinyl neodecanoate and its various pathways into the marine environment;
- reviewing the various controls to limit discharges, emissions and losses of vinyl neodecanoate;
- assessing the extent of the risk posed by vinyl neodecanoate to the marine environment;
- assessing what further activities should be undertaken by OSPAR, or other relevant international organisations, in order to achieve the various OSPAR commitments.

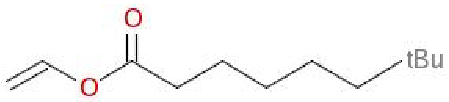
This Background Document takes into account the “Interim Guidance on how to address Hazardous Substances for Priority Action” agreed at OSPAR 1999 (cf. Annex 7 of the Summary Record OSPAR 99/15/1) and follows the general structure for OSPAR background documents outlined in that document.

Vinyl neodecanoate has undergone a hazard assessment in the OECD SIDS assessment programme, and has more recently undergone detailed risk evaluation (including the marine compartment) by the Environment Agency as part of the UK Co-ordinated Chemicals Risk Management Programme, following the assessment methodology of the EU Existing Substances Regulation (EC) no. 793/93 (ESR). Much of the information used here is taken from the final agreed OECD assessment and this Environment Agency evaluation. The UK Environment Agency risk evaluation is a final draft and was not publicly available at the time of the publication of this background document; the draft can be electronically accessed through the list of references at the back of the background document.

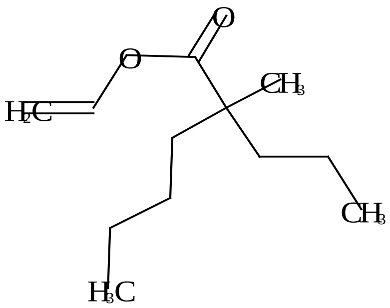
2. Identification of all sources of the substance and pathways to the marine environment

2.1 Properties of vinyl neodecanoate

This assessment considers the following commercial substance:

CAS Number:	51000-52-3
EC Number	256-905-8
IUPAC Name:	ethenyl 6-*tert*-butylhexanoate (registered structure)
Molecular Formula:	$C_{12}H_{22}O_2$
Molecular Weight:	198.31
Synonyms:	Vinyl neodecanoate, vinyl versatate, neodecanoic acid vinyl ester, neodecanoic acid ethenyl ester, trialkyl acetoxy ethane, vinyl ester of Versatic 10, VeoVa10.
SMILES Code	O=C(OC=C)CCCCCC(C)(C)C
CAS Registered Structure	

NOTE: Vinyl neodecanoate is a mixture of structural isomers as a result of the alkyl chain branching of the neodecanoic (versatic) acid component, but always contains a tertiary carbon atom alpha (α) to the carbonyl (VeoVa 10 Data Sheet, 1988). Originally the structure of the substance was registered under CAS number 51000-52-3 as having a saturated straight chain bonded to the carbonyl with a terminal tertiary butyl group, as above. However this structure is not representative of the supplied substance. An example commercially-relevant structure of the substance as manufactured is given below. (Note that the example structure does not include further branching patterns in the R1 and R2 groups, although it seems that such patterns are possible and likely from the versatic acid feedstock used in manufacture of the substance).

Structural Formula:	CH_2=CH-O-CO-C(CH_3)(R^1)(R^2) where R^1 and R^2 = sat. C_7H_{16} in a variety of branching patterns (VeoVa 10 Data Sheet, 1988)
Representative SMILES Code of supplied product	C=COC(=O)C(C)(CCC)CCCC
Example structural formula	 in this structure R^1 = n-butyl and R^2 = n-propyl

Vinyl neodecanoate is very toxic to aquatic organisms, based on current test data does not degrade readily in the environment and accumulates in fish (BCF>100). The detailed properties of vinyl neodecanoate, including numerical values for toxicity, persistence and bioaccumulation are set out in the fact sheet at Annex 1, which has been updated from the publicly available version to include data from the OECD hazard assessment (OECD 2007) and some discussion from the draft Environment Agency risk evaluation.

2.2 Identification of sources of vinyl neodecanoate

The only known EU manufacture of the substance occurs at one site situated in a coastal region in the Netherlands.

The only identified use of vinyl neodecanoate is as a reactive monomer in the manufacture of polymer latex emulsions. In the 2007 OECD hazard assessment, industry stated that no known “as such” uses of the substance exist. Processing of the substance is conducted at sites other than the site of manufacture.

2.3 Pathways to the marine environment

Vinyl neodecanoate may reach the marine environment via waste water as a result of industrial processing to form polymers. In addition, residual levels of the substance will be present in polymer latex batches and the products they are used to make, although likely to be at a very low level. Therefore downstream formulation of these batches and use of end products may result in exposure to the marine environment via waste water.

In the 2007 OECD hazard assessment, Industry stated that releases of the substance to the marine environment from its manufacture do not occur, which is described as a dry, continuous process.

3. Quantification of sources

Figure 1 below summarises the various steps in the life cycle of vinyl neodecanoate that may result in releases to the environment, as modelled in the Environment Agency risk evaluation.

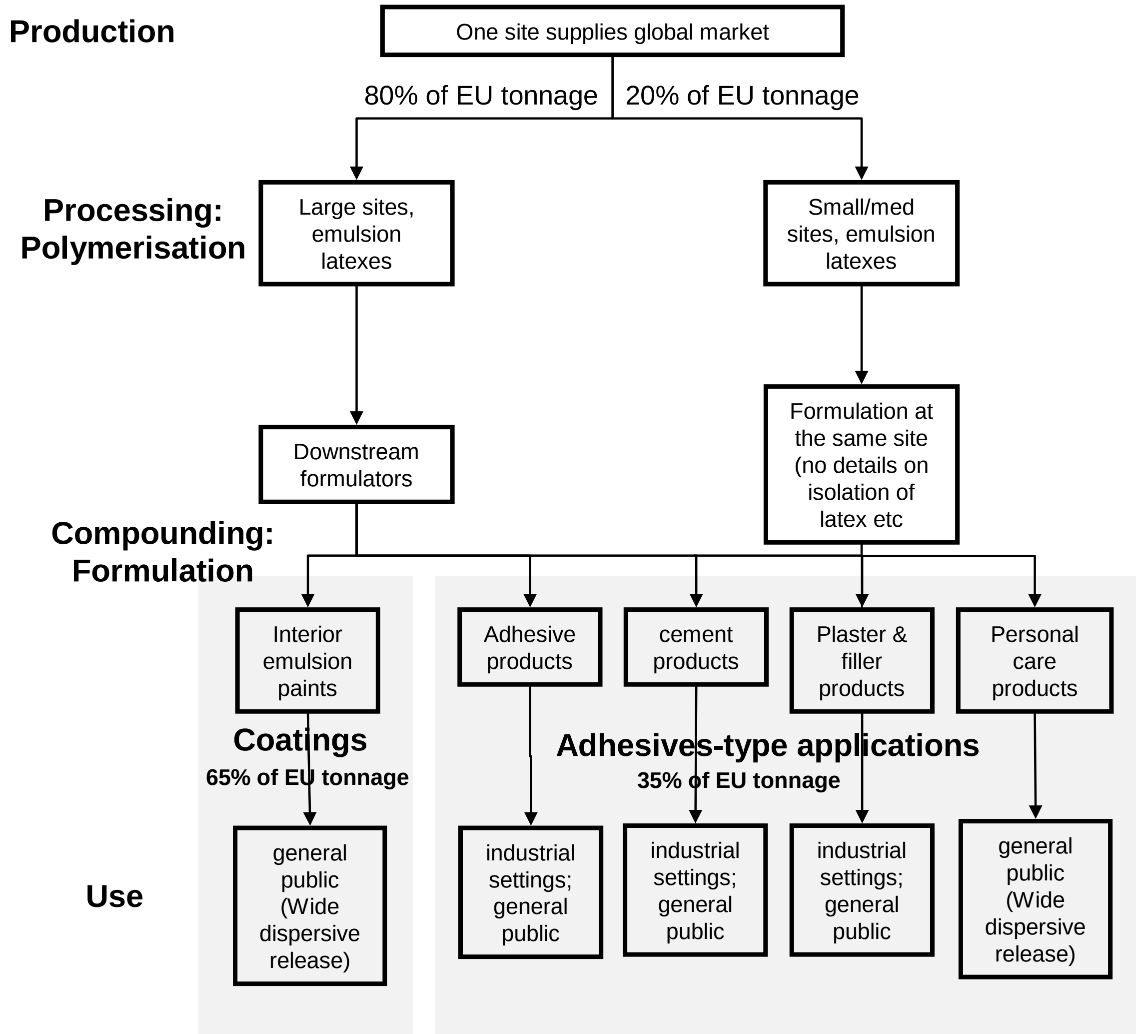


Figure 1: Summary of vinyl neodecanoate and its resulting polymers' use patterns

3.1 Manufacture of vinyl neodecanoate

Vinyl neodecanoate is the ester derived from the reaction of versatic acid (neodecanoic acid) and acetylene, using a zinc salt catalyst (usually a zinc carboxylate i.e. a versatic salt in this case) at elevated temperature. Versatic acid is a mixture of highly branched C10 monocarboxylic acids obtained by the Koch process, which involves the addition of carbon monoxide in the presence of water to a branched terminal alkene. The reaction is catalysed by a mineral acid and usually requires high temperature and pressure. Industry have described the process as being dry, and occurring continuously over 365 days per year (OECD SIDS, 2007).

The annual global production volume of vinyl neodecanoate in 2006 was between 46 and 230 kilotonnes (OECD SIDS, 2007).

According to the major industry supplier of vinyl neodecanoate, it is produced at one site in the EU in the Netherlands that supplies the global market. According to the EU Technical Guidance Document for the risk assessment of chemicals (2003), the production of vinyl neodecanoate falls under the industry category “03 Chemical Industry: chemicals used in synthesis” and the use category “33 Intermediates”.

Industry information suggests that in 2003, 29,000 tonnes of vinyl neodecanoate was sold in the EU and all of this polymerised into latex. More recent information (OECD SIDS, 2007) suggests this figure may be significantly higher now (57% of total production tonnage). In the UK in 2001, 5400 tonnes (18.6% of the EU market) of vinyl neodecanoate was imported for processing, with 99% of this volume being processed at five different sites (Resolution Performance Products, 2002).

Information on importation of the substance from outside the EU, either itself or as a residual component of polymer latex, is not available but thought not to occur.

3.2 Quantification of uses

To the best of the Industry’s knowledge, vinyl neodecanoate is used entirely as a synthetic intermediate in the production of polymeric binding agents for use in latex (water-dispersed polymer) coatings, commercially called “Veocryls” (OECD SIDS, 2007). There is some indication that this categorisation also includes use in adhesives. Solvent-borne vinyl neodecanoate-based polymers and powders can also be produced, however. An exhaustive search of the publicly available literature (Science Information Services, Environment Agency, 2008a-e) found no examples of the substance being used as such (unreacted). Generally vinyl neodecanoate is employed as a co-, ter- or higher monomer, in that it is polymerised with at least one other monomer to give a polymeric material consisting of mixed monomer units (generally the words “co-monomer” and “co-polymer” are used here for simplicity).

Industry have stated that approx. 57% of the global production of vinyl neodecanoate is sold in the EU. Taking the upper limit of production of 230,000 tonnes, this equates to 131,100 tonnes (the lower limit would give 26,220 tonnes). Industry have also stated that all of this is polymerised into latex to the best of their knowledge. In the Environment Agency evaluation the assumption is made that almost all vinyl neodecanoate will be reacted according to the emulsion polymerisation process, given the nature of the final products that contain co-polymers made from vinyl neodecanoate.

Co-polymers containing the polymeric material made from vinyl neodecanoate have a range of uses which can generally be described as coatings and adhesives. The major use falls under the coatings category (65%). Specific uses for VeoVa-based polymers (vinyl neodecanoate is sometimes called VeoVa-10 commercially, short for vinyl ester of Versatic 10; the number denotes number of carbons. Other VeoVa monomers are available) include emulsion paints (indoor and outdoor), solvent-borne metal topcoats, architectural coatings (for wood, metal, roof tiles and concrete), decorative plasters, cement mortar additives and cement composites (including spray-dried powders), solution polymers for various applications (including automotive and industrial coatings and cosmetics), fuel additives, and various powder coatings (Resolution Performance Products, 2002d). There is a trend towards (organic) solvent-free and low volatile organic content (VOC) paints for environmental and human health reasons, and so latex coatings made from vinyl neodecanoate polymers and other emulsion polymers seem to be increasingly used for such applications.

For each application the form of the polymer, and therefore synthetic procedure, is dependent on the downstream formulations or uses. For example, polymers can be formulated for use in a product as an aqueous dispersion, generally involving the use of a latex formed from emulsion polymerisation; re-dispersible and spray-dried polymeric powders may be derived from polymers produced by bulk or suspension polymerisation; or products containing an organic solvent-borne polymer may be formulated using a polymer dispersed in a suitable organic solvent produced by solution polymerisation.

Based on industry information, emulsion polymerisation is believed to be far and away the biggest method for producing co-polymers from vinyl neodecanoate and co-monomers. This process is commonly employed to produce latexes for emulsion paints, adhesives, primers and sealers in which the polymer particles are small (100 – 250 nm diameter) (Resolution Performance Products, 2002c). Table 1 below gives a typical "recipe" for emulsion polymerisation (taken from several sources including Resolution Performance Products, 2003 and Howarth and Hayward, 1996).

Table 1: Typical Quantities of Ingredients Used in Emulsion Polymerisation

Chemical	Function	Approx. relative quantity (%)
Water	Continuous phase	55
Methyl methacrylate	Monomer	17
Vinyl neodecanoate	Monomer	27
Butyl acrylate	Monomer	0.3
Anionic surfactant	Stabilizer	0.3
Hydroxyethyl cellulose	Protective colloid	0.3
Potassium persulfate	Free Radical initiator	0.3

In a communication to the Chemical Stakeholder Forum (Resolution Performance Products, 2002), industry stated that the range of vinyl neodecanoate in a copolymer was 5 – 40%, with 20% being typical.

Vinyl neodecanoate is co-polymerised with vinyl acetate and often an additional "soft" acrylate (for example 2-ethyl hexyl acrylate or butyl acrylate) according to the emulsion polymerisation technique to produce lattices for solvent-free paints. This latex is then formulated in one or more further steps to produce the final blended emulsion paint. These paints are complex mixtures containing the emulsion polymeric materials, pigments, plasticizers, and various additives: additional dispersants, wetting agents, defoamers, thickeners and biocides. They are generally used for interior applications, for example as matt interior paints and silk paints (Hexion Specialty Chemicals, 2006b). In the UK co-polymers of vinyl acetate/vinyl neodecanoate are said to have the largest usage for this application, although co-polymers made from vinyl acetate and acrylic monomers also feature strongly (Howarth and Hayward, 1996).

The Environment Agency risk evaluation assumed that two main scenarios were in use for the polymerization of vinyl neodecanoate based on information reported for the related reactive monomer vinyl acetate (which is often used as a co-monomer with vinyl neodecanoate) (see figure 1). The first scenario is large scale polymerization accounting for 80% of the supplied volume of vinyl neodecanoate, with formulation of the latex polymer into products occurring at separate sites. The second scenario is small scale, specialist polymerization accounting for the remaining 20% of the supplied volume of the substance, with formulation into products likely to occur at the same site.

In the literature emulsion polymerisation is accepted to proceed to over 99% conversion, with most emulsions containing less than 0.5% unreacted monomer. Specific information according to Industry on vinyl neodecanoate is that emulsion polymerisation is carried out in two batchwise stages, with the emulsion containing less than 0.05% unreacted vinyl neodecanoate after the first stage and between 0.01 – 0.02% unreacted vinyl neodecanoate after the second stage (BCF, 2002; OECD SIDS, 2007). In the Environment Agency risk evaluation, the fraction of unreacted vinyl neodecanoate in the final emulsion is taken to be at the higher end of this range, 0.02%, in this assessment.

The copolymer latex produced from polymerization is handled in a formulation step, referred to here as compounding, to produce ready-to-use products such as paints and adhesives. Depending on the type of facility carrying out the compounding and the envisaged use of the final product, the actual formulation process and possible emission patterns from it are likely to vary. It is not clear from the available information if compounding occurs at the same sites as polymerization for vinyl neodecanoate, but some assumptions have been made based on data for vinyl acetate (see above).

A "worst case assumption" would be that all of the residual monomer from emulsion polymerisation remains in the emulsion during and after downstream user formulation into paints and coatings. This assumption may be justified as the emulsion will not be exposed to extremes of temperature or other physical conditions that might invoke substantial decomposition of the residual monomer, as such changes would affect the stability of the emulsion. Industry have indicated that the proportion of unreacted vinyl neodecanoate in finished emulsion paints is typically in the region of 0.006%. If a 3 – 4 fold dilution was employed as part of the formulation process this would result in roughly the residual vinyl neodecanoate concentration reported by industry (from a "stock" emulsion containing 0.01 – 0.02% unreacted vinyl neodecanoate). Industry information for the UK (BCF, 2002) states that coatings contain 5 – 40% emulsion depending on the particular use, with 20% being typical, so this assumed dilution seems reasonable (equating to a concentration of 25 – 33%).

Industry have indicated that the relative quantity of polymer emulsion used for emulsion paints is 65% of the total production (OECD SIDS, 2007). In a communication to the Chemicals Stakeholder Forum (Resolution Performance Products, 2002), Industry stated that the main application of vinyl neodecanoate-based polymers was in decorative paints in the UK (with use in industrial adhesives less than 5%). In the Environment Agency risk evaluation, which considers the EU, the former data have been used - a fraction of 0.65 of the 655,500 tonnes of polymer emulsion (i.e. 426,075 tonnes) is assumed to be formulated into paint.

Vinyl neodecanoate co-polymers may be used in water-borne undercoats and topcoats for exterior wood application, although this is thought to be a low volume specialist use. Primarily this usage is driven by the move away from high-VOC solvent-borne paints. However exact figures for this use are not available as manufacturers often only specify "VeoVa" as one of the polymer components, but not specifically which type of "VeoVa" (i.e. "VeoVa 10" refers to vinyl neodecanoate, whereas "VeoVa 9" and "VeoVa 11" refer to the homologous monomeric materials with nine and 11 carbon atoms, respectively).

Information in the public domain describing products containing vinyl neodecanoate co-polymeric materials include a variety of masonry paints and anti-corrosives coatings (Science Information Services, 2008c). No information on quantities that are used for this purpose are available. It appears that the majority of these are, as for the other coatings applications, aqueous dispersions. Annex I of the Environment Agency report lists a selection of suppliers and trade names, and descriptions where available.

Polymer latexes made using vinyl neodecanoate as one of the monomers that are not formulated into coatings or paints may also be used in adhesives as the binding material. This paragraph describes several types of adhesive most likely to include such co-polymeric materials. The main types of adhesive by mode of action are pressure-sensitive adhesives (PSA) and related contact adhesives, hot-melt adhesives, solution adhesives (including solvent-based and water-based solution adhesives) and structural or reactive adhesives (including epoxy, acrylic, urethane and phenolic adhesives) (see also Kirk-Othmer Encyclopedia of Chemical Technology, J Wiley and Sons; Ohm, R., Ed, 1990; Skeist, I., Ed 1977). In PSAs that are water-based, aqueous emulsions of these same polymers can be used. One example in the public literature exists in which a vinyl acetate, ethylene and VeoVa (chain length not stated) polymer is used as a contact adhesive (Mowilith LDM 1355, manufactured by Celanese; see Annex I of the Environment Agency risk evaluation). It seems likely that vinyl neodecanoate polymers are not widely used in this area. Hot-melt adhesives are solids that require heating before application, and cure upon cooling. It is possible that some resins used for this purpose may be based on a copolymer system including polymerised vinyl neodecanoate. In the public domain at least two companies manufacture a copolymer dispersion used as a heat-seal/melt adhesive (Celanese, vinyl acetate-ethylene-vinyl neodecanoate polymeric material "Mowilith LDM 1025"; Vinavil, poly vinyl acetate-vinyl versatate polymerics "Vinavil 1515" and "Ravemul 023"; see Annex I of the Environment Agency risk evaluation). Solution adhesives can be organic solvent or water-based. No specific information on the use of vinyl neodecanoate copolymers in solvent-based solution adhesives has been identified. For water-based solution adhesives there is the possibility that vinyl neodecanoate copolymers may be used. In the public domain several examples of such uses of vinyl neodecanoate polymers are available: vinyl acetate, ethylene and VeoVa co polymeric materials (as for hot-melt adhesives), acrylate-vinyl acetate-VeoVa polymers from manufacturer Collano and styrene-vinyl acetate-vinyl versatate polymeric materials produced by Neste Chemicals (see Annex I of the Environment Agency risk evaluation). In summary, copolymers made using vinyl neodecanoate as one monomer may be used as binders in hot-melt and water-based solution adhesives primarily, with limited use in PSAs.

Polymers can be added to cement to strengthen and/or modify the concrete matrix. Addition of emulsion polymers also helps the adhesive properties of the cement (Arcozzi *et al.*, 1997). There are three kinds of polymer-based admixtures (also known as cement modifiers). These are polymer-modified mortar, polymer mortar and polymer-impregnated mortar/concrete. The first of these includes copolymers based on vinyl neodecanoate-vinyl acetate. Other co-polymer systems used are based on vinyl acetate-ethylene-vinyl neodecanoate, vinyl acetate-VeoVa-acrylate, vinyl acetate-vinyl versatate-maleic ester and vinyl acetate-vinyl versatate-acrylate-ethylene monomer mixes. The proportion of polymers which incorporate vinyl neodecanoate for this purpose is unknown, but some commercially available examples exist (see Annex I of the Environment Agency risk evaluation). This is thought to be a minor use of these latex polymers.

In decorative plasters and fillers, emulsions of vinyl neodecanoate copolymers can be used as the vehicle and/or binding agent. Plasters and fillers differ from cement in that they are soft and can be manipulated after drying. Information in the public domain describing plaster products containing vinyl neodecanoate co-polymeric materials include a variety of renders and plasters for use in architecture (e.g. Polyfilla Fine Surface™). Unlike acrylic fillers, vinyl emulsion fillers can be dissolved in water after drying (Craft and Solz, 1998). Annex I lists a selection of suppliers and trade names, and descriptions where available. From the available information, it seems that plasters and fillers that incorporate a polymer made from vinyl neodecanoate are more likely to be used by professionals than the general public. As for cements, this is thought to be a minor use of these latex polymers.

Polymers made from vinyl neodecanoate have been used in several types of personal care product including hair sprays, styling products, shampoos and body washes. These are emulsion copolymers based on vinyl acetate-crotonate-vinyl neodecanoate and acrylate-vinyl neodecanoate monomer mixes. The former copolymer is used in hair sprays (at 2% by weight in the one hair spray to give relative constituent proportions), and the latter copolymer at 4.2 – 7% by weight in shampoos and body washes. However this appears to be a specialist and likely low volume use.

4. Monitoring data on discharges, emissions and losses

4.1 Aquatic inputs to the marine environment

No data are available on loads of vinyl neodecanoate entering the OSPAR Convention Waters and the Greater North Sea.

4.2 Atmospheric inputs

No data are available on atmospheric inputs of vinyl neodecanoate into the marine environment but considering its moderate to high vapour pressure the potential exists, depending on venting practices employed during the manufacture and polymerisation of the substance.

4.3 Concentrations in the marine environment (and other waters/sediments)

There are no available measured levels of vinyl neodecanoate in marine waters, estuarine sediments, freshwaters, freshwater sediments or waste waters.

4.4 Concentrations in biota

There are no available data on the levels of vinyl neodecanoate in biota.

5. Assessment of the extent of the problem

5.1 Introduction

In order to assess the extent of the problem, a marine risk assessment based on the guidance developed by OSPAR and the EC in recent years was recently carried out as part of the Environment Agency risk evaluation of the substance. The Marine Risk Assessment involved two steps. Firstly, the preparation of a PBT assessment to ascertain whether the substance is so hazardous that measures should be developed solely on the basis of the information available on sources and pathways to the marine environment. This was followed by a more traditional risk assessment approach where the predicted environmental concentrations were compared with the predicted no effect concentrations to give a PEC/PNEC ratio for various scenarios. The PEC/PNEC ratios give a numerical indication of the degree of risk. The details of the marine risk assessment are summarised here (and can be found in the Environment Agency risk evaluation in section 5.5 of the report). The marine risk assessment draws on data and information in the OECD Hazard assessment. It is clear that the marine risk assessment would be greatly improved with the provision of better quality information.

5.2 PBT Assessment

Criteria for persistency (P), bioaccumulation (B) and toxicity (T) are considered both within the OSPAR context and the REACH Regulation (EC) No. 1907/2006. However the criteria are slightly different, as summarised below.

	OSPAR	**REACH**
Persistent (P)	Half-life ≥50 days	Half-life >60 days (marine water) >40 days (fresh/estuarine water) or >180 days (marine sediment) or >120 days (freshwater/estuarine sediment or soil)
Very Persistent (vP)	Not applicable	Half-life >60 days (fresh/estuarine/ marine water) or >180 days (freshwater/estuarine sediment or soil)
Bioaccumulative (B)	Log Kow ≥4 or BCF ≥500 l/kg	BCF >2,000 l/kg
Very Bioaccumulative (vB)	Not applicable	BCF >5,000 l/kg
Toxic (T)	Acute $L(E)C_{50}$ ≤1 mg/l or long-term NOEC ≤0.1 mg/l or CMR[1] or chronic mammalian toxicity	Long-term NOEC <0.01 mg/l or CMR or chronic mammalian toxicity

An assessment of vinyl neodecanoate against the criteria used under REACH is available in the Environment Agency risk evaluation. In summary:

Persistence: No measured data relating to degradation in the freshwater or marine environment are available for vinyl neodecanoate. Available laboratory studies conducted according to OECD test guidelines (301D and 302C) show that the substance is neither readily nor inherently biodegradable. Although there are uncertainties associated with these tests (and especially the inherent test; see section 3.2.2 of the Environment Agency report), and QSAR predictions indicate that the substance should biodegrade rapidly, in the absence of further test data the “P” screening criteria are fulfilled.

Bioaccumulation**:** The measured octanol-water partition coefficient of vinyl neodecanoate suggested that the “B” screening criteria were met. A bioaccumulation study in fish following a protocol in which the substance was dosed via food was conducted. This study resulted in a biomagnification factor of 0.137. Using the depuration data to estimate a BCF involved estimating what the uptake rate constant would have been had the substance been tested via water exposure. According to the method of Sijm *et al.* (1995), an estimated uptake rate constant resulted in a bioconcentration factor in the range of 1100 – 1670. Other methods are available to estimate uptake rate constants, some resulting in higher estimates of bioconcentration with BCFs >2000. However there is a great deal of uncertainty attached to this estimation approach. On balance, considering the food assimilation efficiency, depuration rate and half life that were measured directly in the feeding study, it can be concluded that the substance is unlikely to meet the “B” (or “vB”) criteria.

Toxicity**:** No long term studies are available (the criterion used is a long term NOEC of <0.01 mg/l). The available laboratory data indicate that invertebrates are the taxonomic group most sensitive to vinyl neodecanoate; two acute studies have been conducted with the marine copepod *Acartia tonsa* (Girling *et al*., 1991; Worden *et al*., 2001). The former indicated that the EC50 ranged between 0.06 and 1.3 mg/l, the latter gave an EC50 of 0.3 mg/l and a NOEC of 0.11 mg/l. In both studies variable analytical recoveries were recorded. These were more marked in the Girling *et al*. study, which was not conducted to GLP. Given the shortcomings with this study (most likely owing to the physico-chemical properties of the substance) it is questionable whether the “T” screening criteria are truly fulfilled. As a precautionary approach and in the absence of confirmatory chronic test data, the substance is considered to meet the “T” screening criteria.

Studies relating to potential human health risks indicate that the substance has a low degree of toxicity.

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[1] Carcinogenic, mutagenic or toxic to reproduction

No information on the possible effects of vinyl neodecanoate on the endocrine system is available.

In summary, vinyl neodecanoate meets the screening criteria for T in the absence of chronic toxicity data and, in the absence of further information on biodegradation as a precautionary assessment, the persistence screening criteria, for the PBT assessment REACH criteria. Although the measured BCF value is around 80% of the threshold B value, the value is considered a realistic worst case given the other information available (substance half life in fish). Overall, vinyl neodecanoate is not considered to meet the REACH PBT criteria.

However, based on the same data set, the following conclusions are drawn when comparing the properties of vinyl neodecanoate against the OSPAR PBT criteria:

> ***Persistence***: No measured data relating to degradation in the marine environment are available. Available OSPAR “level 2” laboratory studies conducted according to OECD test guidelines (301D and 302C) show that the substance is neither readily nor inherently biodegradable. Although there are uncertainties associated with these tests (and especially the inherent test; see section 3.2.2 of the Environment Agency report), and QSAR predictions indicate that the substance should biodegrade rapidly, in the absence of further confirmatory test data the substance is considered to meet the “P” criterion.
>
> ***Bioaccumulation***: The measured octanol-water partition coefficient of vinyl neodecanoate suggested that the “B” screening criteria were met. A bioaccumulation study in fish following a protocol in which the substance was dosed via food was conducted. This study resulted in a biomagnification factor of 0.137. Using the depuration data to estimate a BCF involved estimating what the uptake rate constant would have been had the substance been tested via water exposure. According to the method of Sijm *et al.* (1995), an estimated uptake rate constant resulted in a bioconcentration factor in the range of 1100 – 1670. Other methods are available to estimate uptake rate constants, and all of these returned BCF estimates >500. However it should be noted that there is uncertainty attached to these estimation approaches. On balance, considering the direct results of the feeding study and the QSAR-estimated BCFs for the substance, it can be concluded that the substance meets the “B” criterion.
>
> ***Toxicity***: No long term studies are available. The available laboratory data indicate that invertebrates are the taxonomic group most sensitive to vinyl neodecanoate; two acute studies have been conducted with the marine copepod *Acartia tonsa* (Girling *et al.*, 1991; Worden *et al.*, 2001). The former indicated that the EC50 ranged between 0.06 and 1.3 mg/l, the latter gave an EC50 of 0.3 mg/l. In both studies variable analytical recoveries were recorded; these were more marked in the Girling *et al.* study. Based on the preferred Worden *et al.* study, the T criterion is met.

It is clear that the potential persistence of vinyl neodecanoate is critical for the OSPAR PBT assessment of the substance, because both the available ready and inherent tests have shortcomings that add uncertainty to concluding on the substance’s persistence. This uncertainty is compounded by the QSAR predictions that suggest the substance will biodegrade rapidly.

Hence there is an urgent need to further investigate the substance’s persistence, using a test that is appropriate for the substance’s properties of low water solubility, adsorption and volatility. A modified inherent biodegradation test may be suitable according the OSPAR “level 2” data requirements, otherwise a “higher tier” test might be required.

Until further work on persistence is available to show otherwise, vinyl neodecanoate is considered to meet all three of the OSPAR criteria for the PBT assessment.

5.3 PEC/PNEC ratios for the local marine risk assessment

The PNEC for marine waters of 0.03 µg/l is derived from a test involving the most sensitive organism tested with vinyl neodecanoate. Equilibrium partitioning is used to derive a PNEC for marine sediment from this result: PNECmarine sediment = 7.67 µg/kg wet wt. Comparing the marine PECs with these PNECs gives the risk characterisation ratios listed in table 2. PEC/PNEC ratios for marine secondary poisoning are also presented (for details of the derivation of the PECs and PNECs and the various assumptions which have been used, see the Environment Agency report). There are potential risks for aquatic organisms (including sediment) for the compounding (polymerisation) of vinyl neodecanoate and for the release of residual concentrations of the monomer contained in latex emulsions formulated into paints and adhesives. These risks are based on worst case assumptions in the absence of further specific data on environmental concentrations, and so may be overly conservative. One risk for secondary poisoning in the marine environment is indicated.

Further details of the marine risk assessment can be found in the Environment Agency draft risk evaluation (section 5.5 therein).

Table 2: Estimated PEC/PNEC ratios for vinyl neodecanoate for the local marine risk assessment and secondary poisoning

Lifecycle stage	Step/type	PEC/PNEC ratios for marine water and sediment	PEC/PNEC ratios for marine predators	PEC/PNEC ratios for marine top predators
Production	-	0.14 [a]	2.24×10^{-4} [a]	2.11×10^{-4} [a]
Processing	Large scale processors	**2230**	**1.38**	0.275
	Small/med scale processors	**145**	0.0898	0.018
Use in coatings – emulsion paints	Formulation	**94.4**	0.058	0.012
	Private use	0.233	2.68×10^{-4}	2.2×10^{-4}
Use in adhesives	Formulation	**508**	0.314	0.063
	Private use	0.164	2.25×10^{-4} [a]	2.13×10^{-4} [a]
Use in cements	Formulation	**1.47**	1.03×10^{-3}	3.75×10^{-4}
	Industrial use	0.723	2.7×10^{-4}	2.23×10^{-4}
Use in plasters/fillers	Formulation	**1.69**	1.17×10^{-3}	4×10^{-4}
	Industrial use	0.723	2.7×10^{-4}	2.23×10^{-4}
Use in personal care products	Formulation	0.142 [a]	2.12×10^{-4} [a]	2.11×10^{-4} [a]
	Private use	0.14 [a]	2.11×10^{-4} [a]	2.11×10^{-4} [a]

[a] PEC/PNEC ratios for these scenarios approach those at the regional level, i.e. local releases are almost zero.

5.4 Conclusion of the Risk Assessment for the marine compartment

Some of the indicated risks for marine water and sediment are very high. The PNECs for marine waters and sediment are low (conservative), based on a sensitive marine species and using a high assessment factor (10,000) in accordance with the EU TGD.

For the marine water assessment, more information on the location and releases of sites processing the substance and sites formulating the co-polymer latex containing unreacted vinyl neodecanoate is required. The marine assessment assumes that waste water from industrial sites enters the marine environment with minimal or no pre-treatment, in contrast to the freshwater assessment. If any sites for which risks are identified are located in coastal regions then information on the quantities of the substance in waste water and their practices for disposing of it would be very useful, especially in the case of processors who polymerise the substance into latex and those that formulate the latex into paints.

Given the conservative approach taken, it is likely that the risks indicated for the other formulation steps (cements and plasters) are “false positives”. (It should be noted that refinement of the emissions for freshwater will have an impact on the marine assessment as it is currently derived.) A single risk for marine predators is identified for the fish food chain. Given this last result’s closeness to 1, it is likely to be a “false positive” for the reasons given above.

The PNEC for the marine environment is derived from the acute Acartia tonsa toxicity data. Further data for the purposes of refining the freshwater assessment would be useful in refining the assessment factor used for the marine aquatic PNEC.

If risks still remain for the marine compartment after this, a long term study in Acartia tonsa (a study similar in nature to the OECD 211 test guideline (Daphnia magna reproduction test)) would add greater certainty to the derivation of the marine water PNEC (and again should allow use of a lower assessment factor). Should risks still remain, a chronic study in another marine invertebrate species could be considered.

For sediment, the refinements for the marine water PNEC would refine the sediment PNEC given that it is derived from equilibrium partitioning. A more reliable value of Koc would help with partition modelling. If a freshwater sediment test was conducted, this information would prove useful to compare the marine sediment PNEC against.

6. Achieving the desired reductions

6.1 OSPAR targets

The OSPAR Strategy with regard to Hazardous Substances sets out that the OSPAR objective with regard to hazardous substances is "*to prevent pollution of the maritime area by continuing to reduce discharges, emissions and losses of hazardous substances, with the ultimate aim of achieving concentrations in the marine environment near background values for naturally occurring substances and close to zero for man-made synthetic substances*."

The timeframe given in the Strategy states that "every endeavour will be made to move towards the target of cessation of discharges, emissions and losses of hazardous substances of concern by the year 2020."

At OSPAR 2002, OSPAR adopted guidance on the role of marine risk assessment, which gives, in particular, advice on the urgency of taking measures based on particular PEC/PNEC ratios (cf. Annex 6 of OSPAR 2002 Summary Record). The UK has attempted to apply this guidance and reached the following conclusions. However, these conclusions are considered to be provisional, and could change in the light of further information which is needed to get realistic estimations of a number of emissions.

The estimated local PEC/PNEC ratios for vinyl neodecanoate for marine water and sediment are greater than 1 for several scenarios, and for a few scenarios are very high. These values will partly reflect the conservative nature of the assessment, but nevertheless indicate that further work to refine the assessment is required.

The guidance recognises, however, that where the uncertainties are high in the estimation of risk, this should be taken into account by the Contracting Parties when considering the actions necessary to achieve OSPAR’s objectives.

In this instance, default values have been used in the calculation of emissions from the various processes, and further exposure information is needed to refine the PEC assessments along with better values for Henry’s law constant and adsorption/desorption coefficient for the purposes of environmental fate and behaviour modelling. Specifically, information on the following would be very useful (and also apply to the refinement of the freshwater assessment):

- Tonnage supplied in the EU
- Confirmation of the particular uses (that fall under the headings “coatings” and “adhesives”)
- Further test data to help with environmental fate and behaviour modeling: Henry’s Law and adsorption/desorption constants, Koc
- Quantities used for the different types of processing (polymerization)
  - information on the number and type of processors
  - information on the location of processors (especially those in coastal regions)
  - information on the technical processes and releases
  - further information on levels of residual substance in polymers
  - information on releases to the atmosphere from processing
- Quantities formulated into paints and adhesives
  - information on the number and type of formulators
  - information on the location of formulators (especially those in coastal regions)
  - information on the technical processes and releases during formulation
  - if use in cement composites does exist, quantities formulated and any information on releases

There is no long-term toxicity information on seawater species and so further testing could potentially revise the PNEC for marine water and marine sediment. However, as stated above in the first instance any further testing for the freshwater compartment may allow refinement of the marine PNECs. The Environment Agency risk evaluation contains a suggested toxicity testing strategy should further information on exposure not remove indicated risks (see section 6 “Further work” of the risk evaluation).

No monitoring data are available for vinyl neodecanoate.

Although it does not meet the PBT criteria of REACH, vinyl neodecanoate is considered to meet the OSPAR PBT criteria in the absence of further data to confirm or otherwise its potential persistence. It is therefore imperative from OSPAR's point of view that further work is undertaken to this end. A suitable “OSPAR “level 2” type inherent biodegradability test or relevant higher tier biodegradation test should be initiated.

6.2 OSPAR's role in achieving the desired targets

In order to meet the targets specified in the OSPAR objective and timeframe, it will be necessary to:

- decide which organisation is responsible and/or best placed for carrying out detailed assessments of release, further testing and/or implementing controls;
- inform the relevant organisation (if OSPAR sees fit) of the OSPAR Ministerial commitments with regard to hazardous substances and the need for action to address OSPAR concerns;
- set up mechanisms for monitoring the compliance with any measures adopted in the relevant forum;
- potentially set up mechanisms to monitor inputs to the marine environment and concentrations in the marine environment and biota.

For a number of the sources of vinyl neodecanoate, OSPAR may not be the most appropriate international body to instigate further controls or to assess whether the controls are practicable or necessary. Therefore, setting and achieving the desired reduction targets will need to be carried out through close co-operation with other international forums.

7. Identification of possible measures

7.1 Review of Existing OSPAR, EU and National Measures

7.1.1 Measures in OSPAR

No measures have been taken to date.

7.1.2 Ongoing activities within the European Union

Vinyl neodecanoate has undergone a hazard assessment under the OECD HPV chemicals programme and recently a draft risk evaluation report has been produced from the OECD document and other information by the Environment Agency. The substance has also been registered under the REACH Regulation, and as part of their submission industry have conducted a Chemical Safety Assessment. However this registration is currently not publicly available, and even when it is parts of it will remain confidential.

7.1.3 National initiatives within some Contracting Parties

The lead country is not aware of any other action being undertaken on vinyl neodecanoate currently.

7.2 Alternatives

One of the guiding principles of the OSPAR Strategy on Hazardous Substances is the principle of substitution (the substitution of hazardous substances or preferably non-hazardous substances where such alternatives are available.)

Substitution has been discussed by various OSPAR subsidiary bodies in the 1999/2000 inter-sessional period. The substitution of hazardous substances used offshore has been addressed in OIC and is an essential element of the measures adopted at OSPAR 2000 with respect to the use and discharge of offshore chemicals.

The UK assessment has not yet revealed any definitive substitutes or alternatives which have been used for vinyl neodecanoate.

Substitution of vinyl neodecanoate by another substance would require consideration of the following:

- that the substitute is less harmful and poses a lower risk;
- the physical behaviour of the substance and thus the nature of the processes used to produce these substances;
- the price differential between any substances and vinyl neodecanoate, based on these processes and resulting performance of the product;
- the efficacy of substitutes and the volumes required.

However, as mentioned earlier in this document related reactive monomers are used commercially that differ from vinyl neodecanoate only in number of carbon atoms in their alkyl chain (commercially these substances are all called Veocryls, and specifically VeoVa-x, where x denotes the number of carbons in the versatic acid feedstock). Conceivably, veocryls with one fewer or one more carbon atom (i.e. VeoVa-9 and VeoVa-11) may prove potential substitutes, but it is likely their properties would not differ so much from vinyl neodecanoate so there may be little value in this.

8. Choice for action/measures

8.1 General considerations

The initial results from the marine risk assessment indicate that there may be concern over the use of vinyl neodecanoate and the latex polymer products it is used to make.

However, it should be noted that the majority of the PEC values are derived from default “reasonable worst case” emission estimates and this should be taken into account in the consideration and timing of any measures. The conclusion of the Environment Agency risk evaluation for the marine environment is that there is a potential risk which should be refined with further information and/or testing. This includes better exposure information to refine the PECs and also, if required, further testing on freshwater aquatic and/or marine organisms to reduce the uncertainties over the PNEC.

There is no indication about the location of any of the sites polymerising the substance into latex polymers in the EU, but it is quite possible that some are in coastal regions. Such information should be sought, together with information on marine releases, and used to refine the marine assessment.

A proper evaluation of the appropriate choices for action, including risk reduction scenarios, can only be made if necessary after the risk assessment has been refined with this further information.

8.2 Action in the EC

To support this process and to ensure that the information in this background document and the conclusions reached by OSPAR are generally taken into account in the approach of the European Community, OSPAR should communicate this background document to the European Commission and the European Chemicals Agency.

8.3 Action within OSPAR

In recognition of the large uncertainties in the estimations of risk made, the relevant industries should be invited to work with Contracting Parties to improve the estimates of emissions, and if necessary, the estimation of PNEC values, to ensure the most effective risk reduction measures can be adopted if required.

In terms of the substance’s persistence, the relevant industries should be invited to work with Contracting Parties to provide further information to allow a definitive conclusion for the PBT assessment.

OSPAR should re-evaluate the risks posed by vinyl neodecanoate when further information has been collected. Any associated measures which might be justified in the light of new findings should be addressed through the background document review process.

8.4 Action in other forums

To ensure that the information in this background document can be considered in the context of other international agreements which deal with hazardous substances, and with which Contracting Parties are associated, OSPAR should send copies of this background document to the appropriate bodies dealing with those agreements and invite Contracting Parties who are parties both to OSPAR and those other agreements to promote action to take account of this background document by those other international bodies in a consistent manner.

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Annex 1: Fact Sheet from List of Substances of Possible Concern updated with information from the OECD Hazard Assessment

Updated information is highlighted in pink.

0	**NAME**	**neodecanoic acid, ethenyl ester**		**VERSION: 2002-04-15**
1	**IDENTIFICATION**			
1.1	*CasNo*	51000523		
1.2	*EINECS/ELINCS*	256-905-8		
1.3	*Synonym*	neodecanoic acid, ethenyl ester		
1.4	*Group/Function*	Neodecanoic acid		
1.5	*Initial selection*	**PBT** NSDB(I),		
1.6	*Prioritised for action*	Date: OSPAR 2001; Lead Country: UK; Background document: OSPAR		
	Parameter	**Value**	**Source/Reference**	**Remarks**
2	**PHYSICAL/CHEMICAL PROPERTIES**			
2.1	*Molecular weight, g/mole*	198,31	QSAR-DK:	
2.2	*Water solubility, mg/l*	5.86E+00	QSAR-DK: EPIWIN 3.02	
		5.9 ± 1.3 mg/L at 20ºC	*de Vette, 2007*	

2.3	*Vapour pressure, Pa*	1.14E+01	QSAR-DK: EPISUITE program MpBpVp v1.40	
		38.6 Pa at 25 ºC	*Smith, 2007 (OECD TG 104)*	*No information on test purity or additives was available.*
3	**ABIOTIC/BIOTIC DEGRADATION PROPERTIES**			
3.1	*Abiotic OH-oxidation t½ d*	3.26E-01	QSAR-DK: EPIWIN 3.02	
3.2	*Photolysis t½d*			
3.3	*Ready Biodegradability*			
3.4	*Halflife*	0.294	QSAR-DK:	
			"Although the chemical has not been tested, the vinyl ester functionality is expected to be resistant to hydrolysis due to the tertiary carbon bonding by a similar rationale as in section…and because of the chemical's low water solubility."	*Expert Judgement conclusion, quoted from OECD SIDS 2007.*
3.5	*Inherent Biodegradability*	17 – 19%	IuclidBiodeg:European Commission, ECB, Existing chemicals, TP 280, I-21020 ISPRA	not inherently biodegradable (<20%). Conducted according to OECD302C. Uncertainties associated with test. Method not suitable for volatile test substances. Tested at concentration above water solubility. DOC analysis showed very low levels from early on in the test.
3.6	*Biodeg-QSAR*	0.6434	QSAR-DK: BIOWIN1	readily biodegradable (>70%)
3.6		2.689	QSAR-DK: BIOWIN3	

3.6			QSAR-DK: Interpretation of BIOWIN1and BIOWIN3	readily biodegradable (>70 %)
3.6		0.8004	QSAR-DK:Environ.Tox.Chem. 18(8): 1763-1768. Environ.Tox.Chem. 19(10): 2478-2485. (Syracuse version of H. Loonen's Simca Fragment linear MITI model.)	readily biodegradable (>70 %)
3.6		0.874	QSAR-DK:Environ.Tox.Chem. 18(8): 1763-1768. Environ.Tox.Chem. 19(10): 2478-2485.(Syracuse version of H. Loonen's Simca Fragment non-linear MITI model)	readily biodegradable (>70 %)
4	**BIOACCUMULATION/BIOCONCENTRATION**			
4.1	*logKow*	5	QSAR-DK: EPIWIN 3.02	high potential for bioaccumulation
4.1		6	IuclidBioacc:European Commission, ECB, Existing chemicals, TP 280, I-21020 ISPRA	High potential for bioaccumulation
4.1		3	Revision of GESAMP Reports and Studies No 17 and 35, London , IMO 1989	Low potential for bioaccumulation
2.4	Partition coefficient n-octanol/water (log value)	4.9	measured value (Webb, 2001)	
4.1		5	SHELL	high potential for bioaccumulation
4.2	*Bcf*	631	QSAR-DK: EPIWIN 3.02	high bioconcentration factor
4.2		15180	IuclidBioacc:European Commission, ECB, Existing chemicals, TP 280, I-21020 ISPRA	Very high bioconcentration factor
	BMF	*0.137*	*Hicks* et al., *2007 in OECD SIDS, 2007*	*Dietary bioaccumulation test in rainbow trout. Estimated BCF from the data = 1100 – 1700.*
5	**AQUATIC TOXIC PROPERTIES**			
5.1	*Acute toxicity algae IC50, mg/l*	26	IuclidAquatox:European Commission, ECB, Existing chemicals, TP 280, I-21020 ISPRA	Toxic(10-100 mg/l)

5.2	*Acute toxicity Acartia tonsa EC50, mg/l*	0.06	European Commission, ECB, Existing chemicals, TP 280, I-21020 ISPRA	Very toxic (<0,1 mg/l)
5.2	*Acute toxicity, Acartia tonsa, EC50, mg/l*	*0.3*	*Worden* et al., *2001*	*Very toxic (1 – 0.1 mg/l)*
5.3	*Acute toxicity fish LC50, mg/l*	1	Revision of GESAMP Reports and Studies No 17 and 35, London , IMO 1989	Very toxic (1-0,1 mg/l)
5.3		14	IuclidAquatox:European Commission, ECB, Existing chemicals, TP 280, I-21020 ISPRA	Toxic(10-100 mg/l)
5.4	*Chronic toxicity daphnia NOEC, mg/l*			
5.5	*Chronic toxicity fish NOEC, mg/l*			
5.6	*Aquatox-QSAR*	0.45	QSAR-DK: Acute Daphnia, Danish EPA Multicase Acute EC50 Daphnia model.	very toxic (01-1 mg/l)
5.6		0.2562	QSAR-DK: Fish NOEC, Lethal Body Burden NOEC mg/l (A:C ratio 10:1) for fish based on EPIWIN 3.02 BCF	toxic (01-1 mg/l)
5.7	*Aquatic toxicity - other species*			
6	**HUMAN TOXIC PROPERTIES**			
6.1	*Acute toxicity*			
6.2	*Carcinogenicity*			
6.3	*Chronic toxicity*			
6.4	*Mutagenicity*			
6.5	*Reprotoxicity*			
7	**EXPOSURE**			

7.1	*Production Volume*	LPVC	IUCLID:	10-1000
7.2	*Use/Industry Category*	BASIC INDUSTRY: BASIC CHEMICALS , PAINTS, LACQUERS AND VARNISHES INDUSTRY , ADHESIVE, BINDING AGENTS, CONSTRUCTION MATERIALS ADDITIVES		Source: IUCLID
7.3	*Use in articles*			
7.4	*Environm.Occur. Measured*			(Compartment)
7.5	*Environm.Occur. Modelled*			(Compartment)
8	**EU-LEGISLATION**			
8.1	*Dir 67/548/EEC (Classification)*		:Annex1, Dir 67/548/EEC	
8.2	*Reg 793/93/EEC (Existing substances)*			
8.3	*Dir 2000/60/EEC (WFD)*			
8.4	*Dir 76/769/EEC (M&U)*			
8.5	*Dir 76/464/EEC (water)*			
8.6	*Dir 91/414/EEC (ppp)*			
8.7	*Dir 98/8/EEC (biocid)*			
9	**ADDITIONAL INFORMATION**			
9.1	*Hazard assessment-OECD*			SIDS assessment published 2007.
9.2	*Other risk assessments*			

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