TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

RESULTS OF THE EVALUATION OF THE PBT/VPVB PROPERTIES OF:

Substance name: Vinyl neodecanoate

EC number: 256-905-8

CAS number: 51000-52-3

Molecular formula: $C_{12}H_{22}O_2$

Structural formula:

CH2=CH-O-CO-C(CH3)(R1)(R2)

where R1 and R2 contain seven alkyl carbons in total

Summary of the evaluation:

The substance is not considered to be a PBT substance. It does not meet the B criteria and does not meet the screening criteria for T. It does meet the screening criteria for P (and vP).

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Vinyl neodecanoate
EC Number: 256-905-8
CAS Number: 51000-52-3
IUPAC Name:
Molecular Formula: $C_{12}H_{22}O_2$
Molecular Weight: 198.31
Structural Formula:

CH2=CH-O-CO-C(CH3)(R1)(R2)

where R1 and R2 contain seven alkyl carbons in total

Note: The SMILES notation provided by the Syracuse Research Corporation's EPIWIN (ver. 3.20) upon entering CAS No. 51000-52-3 is O=C(OC=C)CCCCCC(C)(C)C, which does not correctly reflect the chemical's structure with respect to the position of the tertiary carbon. This is a historical anomaly. A more realistic example SMILES notation is C=COC(=O)C(C)(CC)C(C)CCC.

Synonyms: Vinyl neodecanoate, neodecanoic acid vinyl ester, neodecanoic acid ethenyl ester, trialkyl acetoxy ethane, vinyl ester of Versatic 10, VeoVa10.

Vinyl neodecanoate is the ester derived from the reaction of Versatic acid (neodecanoic acid, a synthetic saturated monocarboxylic acid of highly branched structure) and acetylene. Versatic acid is a mixture of highly branched C10 monocarboxylic acids obtained by the Koch process, which involves the addition of carbon monoxide to a branched olefin. Therefore vinyl neodecanoate is a mixture of structural isomers as a result of this alkyl chain branching of the versatic acid component, but always contains a tertiary carbon atom alpha (α) to the carbonyl.

1.1 Purity/Impurities/Additives

Vinyl neodecanoate is a commercial mixture of isomers defined by the general structural formula above. The majority (98%) of the compound falls within this category. The remaining 2% fall under the category of impurities, which consist of residual products (unconverted starting olefins, light and heavy by-products, impurities present in the starting materials, reagents used in the manufacturing process) not removed by distillation.

Mono-methyl ether of hydroquinone. (CAS No. 150-76-5) is used as an additive at a concentration of 0.005 to 0.008 g/Kg, acting as an inhibitor of self-polymerization (OECD, 2007).

1.2 Physico-Chemical properties

Table 1 Summary of physico-chemical properties

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 KPa	Viscous liquid	
V, 5.2	Melting / freezing point	7.2 ºC	calculated value; US EPA MPBPWIN ver. 1.41
V, 5.3	Boiling point	212 ºC	
V, 5.5	Vapour pressure	38.6 hPa at 25ºC	
V, 5.7	Water solubility	5.9 ± 1.3 mg/L at 20ºC	
V, 5.8	Partition coefficient n-octanol/water (log value)	4.9 at 20 °C	Shake flask method
VII, 5.19	Dissociation constant	Not available	

2 MANUFACTURE AND USES

Not relevant.

3 CLASSIFICATION AND LABELLING

Vinyl neodecanoate is classified as Dangerous for the environment under the Dangerous Substances Directive (67/548/EEC), R50-53: very toxic to aquatic organisms and may cause long-term adverse effects in the aquatic environment.

3.1 Degradation (P)

3.1.1 Abiotic degradation

Hydrolysis

No experimental determination of hydrolysis of the substance has been conducted. The vinyl ester functionality is expected to be resistant to hydrolysis due to the steric hindrance of the tertiary carbon bonding preventing attack at the carbonyl. Hydrolysis is therefore not expected to be a significant degradation process in the environment.

3.2 Biotic degradation

The biodegradation data for vinyl neodecanoate have been reviewed as part of the OECD SIDS programme (OECD, 2007). Several biodegradation tests to OECD guidelines indicate that vinyl neodecanoate is not readily biodegradable. Reliable results after incubating the test substance with activated sludge ranged from 3-5% (OECD 302C) to 14-17% (OECD 301D) of the material being

degraded over a 28-d period. These results confirm that vinyl neodecanoate is a material that it is not readily biodegradable nor inherently biodegradable.

3.2.1 Other information [1]

3.2.2 Summary and discussion of persistence

The results of biodegradation tests indicate that the substance is not readily biodegradable.

3.3 Environmental distribution

3.3.1 Adsorption

3.3.2 Volatilisation

3.4 Bioaccumulation (B)

3.4.1 Screening data[2]

3.4.2 Measured bioaccumulation data[3]

The available bioaccumulation data for vinyl neodecanoate has been reviewed under the OECD SIDS programme (OECD, 2007).

Due to problems with analysis of the test media and reproducibility of the analytical methods when attempting to measure the bioconcentration factor (BCF) of vinyl neodecanoate in fish according to OECD test Guideline 305, a fish feeding study was conducted instead. The method involved offering rainbow trout food spiked with the test substance.

The objective of the study was to determine the half-life (t½, from the elimination rate constant, $k_{depuration}$), the assimilation efficiency (α), the biomagnification factor (BMF; where biomagnification refers to the movement of a chemical through the food chain), the lipid-normalized kinetic biomagnification factor (BMFL), "steady-state" biomagnification factor, and bioconcentration factor (BCF).

Vinyl neodecanoate was directly incorporated into fish food (using acetone) and fed to a treatment group. In a range-finding test two concentrations of test substance, 300 µg/g and 3000µg/g, were used in the feed. For the definitive study a concentration of 1500 µg/l was selected, as this fulfilled

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1 For example, half life from field studies or monitoring data

2 For example, log K_{ow} values, predicted BCFs

3 For example, fish bioconcentration factor

the criteria of exhibiting no toxicity, palatability of feed, and gave analytical reproducibility for measured concentrations in the feed. Hexachlorobenzene (HCB) was added to the treated feed to evaluate the assimilation efficiency (α), as this substance is known to readily bioaccumulate and not depurate significantly. The control fish were fed untreated food (treated only with same amount of acetone used in the treatment group). The test consisted of two phases: uptake (10 days) and depuration (28 days, out of a maximum of 42 d). There was no statistically significant difference between the control fish and treated fish growth rates. The determination of the concentration of test substance, the length of each phase, as well as sampling schedules, were based on the preliminary tests. The limit of detection for the substance in whole fish was 0.163 µg/g and for the fish food was 8.16 µg/g.

Depuration rate and biomagnification factors

The growth corrected depuration rate constant was calculated by subtraction of the growth rate constant from the overall elimination rate constant ($k_{depuration} = k_{overall} - k_{growth}$). The chemical assimilation efficiency (α) was calculated using the equation:

$$\alpha = \frac{C_{0,depuration} \cdot k_{overall}}{F \cdot C_{food}} \cdot \left[1 - \exp(-k_{depuration} \cdot t)\right]$$

Where: F is the feeding rate ($g_{food} \cdot g_{fish}^{-1} \cdot d^{-1}$);

C_{food} is the chemical concentration in the food

The dietary kinetic biomagnification factor (BMF) was calculated as $BMF = F \cdot \alpha \cdot k_{depuration}^{-1}$ and the growth-corrected half-life was calculated as $t_{1/2} = 0.693 \cdot k_{depuration}^{-1}$

The "steady-state" BMF_L was calculated by dividing the "steady-state" concentration [i.e., day 10 uptake whole fish mean measured concentration normalized for fish lipid fraction (i.e., 0.037)] by the mean concentration in the feed normalized for the lipid fraction in treated feed (i.e., 0.17). The "steady-state" BMF_L derived from the above calculation was 0.115 (i.e., 778 µg/g divided by 6,760 µg/g).

Lipid Normalisation

The mean lipid fraction ratio food/fish, where the lipid fraction in fish is divided by the lipid fraction in the diet to obtain the lipid normalization factor, was used to calculate the lipid normalized kinetic and steady state biomagnification factors (BMFL); calculated as BMFL = BMF/L, where L equals the mean lipid fraction ratio food/fish (i.e., lipid normalization factor).

Bioconcentration factor

The bioconcentration factor (BCF) was calculated from the dietary test by the following equations:

(1) $BCF = (Ku \times T_{1/2}) / 0.693$

(2) $Ku = (520 \pm 40) \times W^{-0.32 \pm 0.03}$ [4]

where: Ku = the uptake rate constant (L/kg/d)

$T_{1/2}$ = growth corrected half-life from dietary bioaccumulation test (days)

W = fish weight (grams wet weight) at the end of uptake/start of depuration

Since current categorisations for bioaccumulative materials are based on BCF values, the equation above was developed for the purpose of relating the experimentally derived BMF for a test substance to a BCF.

The final results of the definitive study are shown in Table 2 below. Relevant values are quoted on a whole fish wet weight basis.

Table 2 Results of fish feeding study

Elimination rate constant ($k_{overall}$):	3.03×10^{-1} (days)$^{-1}$
Growth-corrected elimination rate constant ($k_{depuration}$):	2.67×10^{-1} (days)$^{-1}$
Growth-corrected half-life ($t_{1/2}$):	2.60 days
Assimilation efficiency (α):	1.84×10^{-1}
Bioconcentration factor [5] $BCF_{Low\ estimate}$:	1.10×10^{3}
Bioconcentration factor $BCF_{High\ estimate}$:	1.39×10^{3}
kinetic Biomagnification factor (BMF):	2.07×10^{-2}
Lipid-normalized kinetic biomagnification factor BMF_L:	9.41×10^{-2}
Lipid-normalized steady-state BMF_L:	1.15×10^{-1}

Hexachlorobenzene had a net assimilation efficiency of 47% (0.47), similar to the >50% assimilation efficiency noted for this chemical mixed with liquid hydrocarbon test chemicals by the laboratories involved in the development of this biomagnification guideline. The empirical lipid-normalized BMF for HCB was calculated by dividing the mean concentration in whole fish at day

4 Allometric relationship taken from Sijm et al., (1995), Toxicol. Appl. Pharmacol., 131:130-135.

5 Bioconcentration Factors derived from Biomagnification Factors are highly conservative because to determine the BCF it is assumed that the test substance is completely soluble in the water phase. For vinyl neodecanoate this assumption is not valid because the substance is not water soluble to any appreciable degree. In addition, the compound was mostly cleared (i.e., >95%) by the fish by day 14 of depuration. Therefore, the calculated BCF values are highly conservative estimates and possibly inappropriate for use in standard environmental fate models.

10 of uptake normalized for fish lipid fraction (i.e., 0.037) by the mean HCB concentration in the feed normalized for the lipid fraction in treated feed (i.e., 0.17). The empirical lipid-normalized BMF for HCB derived from the above equation was 0.54 (i.e., 289 μg/g divided by 539 μg/g = 0.54). This empirical lipid-normalized BMF value falls within the historical range of 0.5 – 2. The lipid-normalized BMF value for vinyl neodecanoate was 0.115.

While the measured octanol-water partition coefficient (Log Kow or Log P) is 4.9, the bioaccumulation potential from this fish study indicates that vinyl neodecanoate is rapidly eliminated (95% clearance in 14 days depuration, kinetic biomagnification factor 0.09). The assimilation efficiency of the HCB control was 47% (indicating high assimilation and in agreement with historical data), and 18% for vinyl neodecanoate. The data were also used to derive a bioconcentration factor from an equation validated for compounds tested in aqueous-dosed bioaccumulation studies (BCF 1100 - 1390). However, given that vinyl neodecanoate (or neodecanoic acid ethenyl ester) is poorly soluble in water this range is likely to be a conservative estimate.

3.4.3 Other supporting information[6]

3.4.4 Summary and discussion of bioaccumulation

A fish feeding study with vinyl neodecanote indicated that the substance is rapidly eliminated from rainbow trout with 95% clearance in the 14 day depuration period. A lipid-normalized kinetic BMF for whole fish of 0.09 was determined. The BCF was estimated from the study to be 1100-1390.

3.5 Secondary poisoning

4 HUMAN HEALTH HAZARD ASSESSMENT

The mammalian toxicity data for vinyl neodecanoate has been reviewed as part of the OECD SIDS programme and a summary of the main findings of this review is given below in Table 3.

Table 3 Summary of mammalian toxicity data

Test	Species	Results
Acute oral (single dose) studies	Rat	Oral 9 d LD50 > 8850 mg/kg bw
Repeated dose studies – oral exposure	Rat	28 day NOAEL 250 mg/kg bw/d based on specific kidney effects (so called male rat nephropathy) seen at 1000 mg/kg bw/d
Developmental toxicity/ teratogenicity	Rat	OECD 422 study –NOAEL 1000 mg/kg bw per day

[6]For example, measured concentrations in biota

5 ENVIRONMENTAL HAZARD ASSESSMENT

5.1 Aquatic compartment (including sediment)

5.1.1 Toxicity test results

5.1.1.1 Fish

Acute toxicity

The available toxicity data for vinyl neodecanoate have been reviewed and validated under the OECD SIDS programme (OECD, 2007). In a semi-static study carried out according to OECD 203 on rainbow trout, a 100 mg/l water accommodated fraction (WAF) was prepared and this was used to produce the different concentrations used in the test. The results based on measured concentrations were 96h LC50 = 0.84 mg/l, 96h NOEC = 0.59 mg/l.

Long-term toxicity

No data available.

5.1.1.2 Aquatic invertebrates

Acute toxicity

The available toxicity data for vinyl neodecanoate have been reviewed and validated under the OECD SIDS programme (OECD, 2007). In a static study with Daphnia magna, a 100 mg/l water accommodated fraction (WAF) was prepared and this was used to produce the different concentrations used in the test. The results based on measured concentrations were 48h EC50 = 1.8 mg/l, 48h NOEC = 1.5mg/l.

Two studies with the marine copepod Acartia tonsa are available. In the earlier (non-GLP) study, a range of EC50s is reported due to variability in analytical recoveries, 48h EC50 = 0.06 – 1.3 mg/l. A more recent study gave results of 48h EC50 = 0.30mg/l, 48h NOEC = 0.11 mg/l and this is the preferred result since the study was conducted to GLP and there was lower variability of analytical recovery.

Long-term toxicity

No data available.

5.1.1.3 Algae and aquatic plants

The available toxicity data for vinyl neodecanoate have been reviewed and validated under the OECD SIDS programme (OECD, 2007). For a study conducted with Selenastrum capricornutum, a

100 mg/l water accommodated fraction (WAF) was prepared and this was used to produce the different concentrations used in the test. The results based on measured concentrations were 72h ErC50 > 4.8 mg/l, 72 EbC50 = 3.4 mg/l, 72h NOEC (growth rate and biomass) = 0.42 mg/l.

5.1.2 Sediment organisms

5.1.3 Other aquatic organisms

5.2 Terrestrial compartment

5.3 Atmospheric compartment

5.4 Indirect exposure via the food chain

6 PBT AND vPvB

6.1 PBT, vPvB assessment

Persistence: the substance is not readily biodegradable so the screening criterion for P/ vP is met.

Bioaccumulation: a reliable *in vivo* experimental BMF of 0.09 was determined in a fish feeding study. The BCF was estimated from the study to be 1100-1390. Hence the substance does not meet the B (or vB) criterion.

Toxicity: The lowest LC50 is 0.30 mg/L for Acartia tonsa. No chronic toxicity data are available. The screening T criterion is not met.

Summary: vinyl neodecanote does not meet the B or vB criteria, and so is not considered a PBT substance according to the EU criteria. It does not meet the screening criteria for T. It does meet the screening criteria for P.

INFORMATION ON USE AND EXPOSURE

Not relevant as substance is not identified as a PBT.

OTHER INFORMATION

The information used in this report was taken from the following sources:

OECD (2007). OECD SIDS Dossier for Neodecanoic acid, ethenyl ester, CAS No. 51000-52-3.