HYDROGENATED POLYDECENE

(CAS #68037-01-4)

GREENSCREEN® FOR SAFER CHEMICALS (GREENSCREEN®) ASSESSMENT

Prepared by:

ToxServices LLC

Assessment Date: July 8, 2025

Expiration Date: July 8, 2030

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GreenScreen® Executive Summary for Hydrogenated Polydecene (CAS #68037-01-4)

Hydrogenated polydecene is a low molecular weight polymer that is a mixture of branched isomeric hydrocarbons each composed of repeated ten-carbon units (oligomers), ranging from C30 to C60. The oligomer distribution is C30 13–37%, C40 35–70%, C50 9–25% and C60 1–7%. Hydrogenated polydecene is a colorless and viscous liquid at room temperature. It is not soluble in water and its measured log K_{ow} of > 6.5 indicates it may bioaccumulate or is not bioavailable, depending on the log K_{ow} value. The vapor pressure for hydrogenated polydecene indicates that it is unlikely to volatilize. Hydrogenated polydecene is used in industrial manufacturing, metal working fluids, lubricants, and coatings. It is also used as a food additive (glazing agent) and in cosmetic formulations as an abrasive, bulking, and film forming agent. The Cosmetic Ingredient Review (CIR) Expert Panel determined that hydrogenated polydecene is safe for use in cosmetics in the present practices of use and concentrations (up to 59%).

Hydrogenated polydecene was assigned a **GreenScreen Benchmark™ Score of 2** ("Use but Search for Safer Substitutes"). This score is based on the following hazard score:

- Benchmark 2c
    - High Persistence-P + Moderate Group I Human Toxicity (single exposure systemic toxicity-STs)

A data gap (DG) exists for endocrine activity-E. As outlined in GreenScreen® Guidance, Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), hydrogenated polydecene meets requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gap. In a worst-case scenario, if hydrogenated polydecene were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

The Benchmark score of hydrogenated polydecene has changed over time. The original GreenScreen® assessment was performed in March 2025 under version 1.4 criteria and ToxServices assigned a Benchmark 3 (BM-3) score. This BM score is updated to 2 in a subsequent revision due to re-evaluation of its aspiration hazard.

New Approach Methodologies (NAMs) used in this GreenScreen® include *in vitro* tests for genotoxicity, expert-based guidance on evaluating respiratory sensitization, and *in silico* modeling for carcinogenicity, persistence, and bioaccumulation. The quality, utility, and accuracy of NAM predictions are greatly influenced by two primary types of uncertainties:

- Type I: Uncertainties related to the input data used
- Type II: Uncertainties related to extrapolations made

Type I (input data) uncertainties in hydrogenated polydecene's NAMs dataset include absence of/insufficient experimental data for carcinogenicity, respiratory sensitization, and bioaccumulation, and lack of established test methods for respiratory sensitization. Hydrogenated polydecene's Type II (extrapolation output) uncertainties include lack of defined applicability domains for the carcinogenicity structural alerts by ISS in the Danish QSAR database, limitations of *in vitro* genotoxicity assays to mimic *in vivo* metabolic conditions, and lack of consideration of non-immunological mechanisms of respiratory sensitization. Some of hydrogenated polydecene's type II uncertainties were alleviated by the use of *in vitro* test batteries and/or in combination of *in vivo* data.

GreenScreen® Hazard Summary Table for Hydrogenated Polydecene

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS	SnR	IrS	IrE	AA	CA	P	B	Rx	F
						s	r*	s	r*	*	*								
L	**L**	**L**	**L**	DG	**L**	**H**	**L**	*L*	**L**	**L**	*L*	**L**	**L**	**L**	*L*	*H*	*vL*	*L*	**L**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.

GreenScreen® Chemical Assessment for Hydrogenated Polydecene (CAS #68037-01-4)

Method Version: GreenScreen® Version 1.4
Assessment Type[1]: Certified
Assessor Type: Licensed GreenScreen® Profiler

GreenScreen® Assessment (v.1.4) Prepared By:
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Organization: ToxServices LLC
Date: March 13, 2025; June 27, 2025

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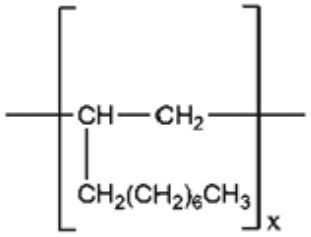
Organization: ToxServices LLC
Date: March 21, 2025; July 8, 2025

Expiration Date: July 8, 2030[2]

Chemical Name: Hydrogenated polydecene

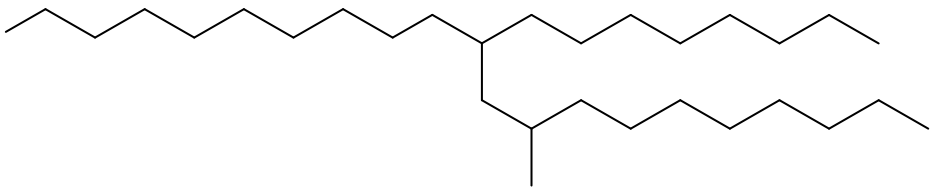
CAS Number: 68037-01-4

Chemical Structure(s):
Hydrogenated polydecene is a low molecular weight polymer that is mixture of branched isomeric hydrocarbons each composed of repeated ten-carbon units (oligomers), ranging from C30 to C60. The oligomer distribution is C30 13–37%, C40 35–70%, C50 9–25% and C60 1–7% (EFSA 2020).



(CIR 2020).

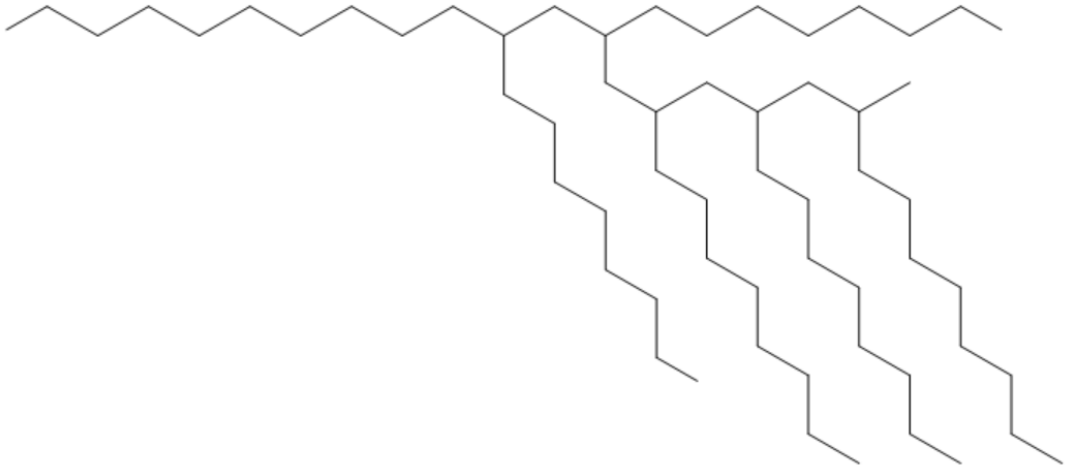
Based on the generic structure above and the description that the smallest oligomer is the trimer of decene that is then hydrogenated (removal of double bond), ToxServices used the following structure, which is the trimer of 1-decene fully hydrogenated, to conservatively represent hydrogenated polydecene in modeling for the carcinogenicity and bioaccumulation endpoints.



SMILES: CCCCCCCCCCC(CCCCCCCC)CC(C)CCCCCCCC

[1] GreenScreen® reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen® Practitioner), or "CERTIFIED" (by Licensed GreenScreen® Profiler or equivalent).
[2] Assessments expire five years from the date of completion starting from January 1, 2019. An assessment expires three years from the date of completion if completed before January 1, 2019 (CPA 2018a).

For persistence and bioaccumulation, the longest constituent, the hydrogenated 1-decene hexamer, was used as a conservative representative of hydrogenated polydecene. The structure of this constituent is shown below.

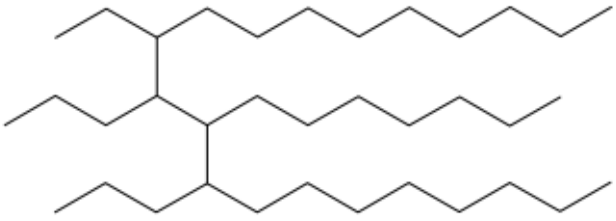


SMILES:
CCCCCCCCCCC(CCCCCCCC)CC(CCCCCCCC)CC(CCCCCCCC)CC(CCCCCCCC)CC(C)CCCCCCCC

Also called:
1-Decene, homopolymer, hydrogenated; Decene, homopolymer; Hydrogenated decene homopolymer (Pharos 2025).

Suitable surrogates or moieties of chemicals used in this assessment (CAS #'s):
Hydrogenated polydecene has a relatively complete toxicological dataset. For the endpoints with data gaps, ToxServices used 1-dodecene trimer, hydrogenated (CAS #151006-62-1) as a surrogate. Both chemicals have been evaluated as a group by the United States Environmental Protection Agency (U.S. EPA) and CIR due to their structural similarity (long-chain branched alkanes, derived from the similar monomer (1-decene, C10 alpha olefin and 1-dodecene, C12 alpha olefin) (U.S. EPA 2010, CIR 2020).

1-Dodecene trimer, hydrogenated (CAS #151006-62-1)



(U.S. EPA 2010)

Identify Applications/Functional Uses: (EFSA 2020, CIR 2020)
1. Glazing agent
2. Release agent
3. Abrasive
4. Bulking agent

5. Film forming agent

Known Impurities[3]:
Hydrogenated polydecene may contain the toxic elements nickel and lead as impurities at acceptable concentrations (up to 1 mg/kg each) (EFSA 2020).

GreenScreen® Summary Rating for Hydrogenated Polydecene[4,5] [6,7]: Hydrogenated polydecene was assigned a **GreenScreen Benchmark™ Score of 2** ("Use but Search for Safer Substitutes") (CPA 2018b). This score is based on the following hazard score:

- Benchmark 2c
  - High Persistence-P + Moderate Group I Human Toxicity (single exposure systemic toxicity-STs)

A data gap (DG) exists for endocrine activity-E. As outlined in GreenScreen® Guidance (CPA 2018b) Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), hydrogenated polydecene meets requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gap. In a worst-case scenario, if hydrogenated polydecene were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

Figure 1: GreenScreen® Hazard Summary Table for Hydrogenated Polydecene

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	**M**	**R**	**D**	**E**	**AT**	**ST**		**N**		**SnS**	**SnR**	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
						s	r*	s	r*	*	*								
L	**L**	**L**	**L**	DG	**L**	**H**	**L**	*L*	**L**	**L**	*L*	**L**	**L**	**L**	*L*	*H*	*vL*	*L*	**L**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.

Environmental Transformation Products
No data on transformation products were identified for hydrogenated polydecene. Due to its insolubility and lack of reactive functional groups, hydrogenated polydecene has reduced susceptibility to hydrolysis and biodegradation of hydrogenated polydecene is not expected to be a significant environmental fate.

Introduction
Hydrogenated polydecene is synthesized by oligomerization of pure 1-decene to the tri-, tetra-, penta- and hexa-decene molecules, followed by hydrogenation to full saturation of the oligomers; both

[3] Impurities of the chemical will be assessed at the product level instead of in this GreenScreen®.
[4] For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.
[5] See Appendix A for a glossary of hazard endpoint acronyms.
[6] For inorganic chemicals only, see GreenScreen® Guidance v1.4 Section 12 (Inorganic Chemical Assessment Procedure).
[7] For Systemic Toxicity and Neurotoxicity, repeated exposure data are preferred. Lack of single exposure data is not a Data Gap when repeated exposure data are available. In that case, lack of single exposure data may be represented as NA instead of DG. See GreenScreen® Guidance v1.4 Annex 2.

processes are carried out in the presence of a catalyst (EFSA 2020). Hydrogenated polydecene is used in industrial manufacturing, metal working fluids, lubricants, and coatings. It is also used as a food additive (glazing agent) and in cosmetic formulations as an abrasive, bulking and film forming agent (EFSA 2020, CIR 2020). The CIR Expert Panel determined that hydrogenated polydecene is safe for use in cosmetics in the present practices of use and concentration (up to 59%) (CIR 2020).

ToxServices assessed hydrogenated polydecene against GreenScreen® Version 1.4 (CPA 2018b) following procedures outlined in ToxServices' SOPs (GreenScreen® Hazard Assessment) (ToxServices 2021).

U.S. EPA Safer Choice Program's Safer Chemical Ingredients List

The SCIL is a list of chemicals that meet the Safer Choice standard (U.S. EPA 2025). It can be accessed at: http://www2.epa.gov/saferchoice/safer-ingredients. Chemicals on the SCIL have been assessed for compliance with the Safer Choice Standard and Criteria for Safer Chemical Ingredients (U.S. EPA 2024a).

Hydrogenated polydecene is not listed on the U.S. EPA's SCIL.

GreenScreen® List Translator Screening Results

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen Benchmark™ 1 chemicals (CPA 2018b). Pharos (Pharos 2025) is an online list-searching tool that is used to screen chemicals against all of the lists in the List Translator electronically. ToxServices also checks the U.S. Department of Transportation (U.S. DOT) lists (U.S. DOT 2008a,b),[8] which are not considered GreenScreen® Specified Lists but are additional information sources, in conjunction with the Pharos query. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for hydrogenated polydecene can be found in Appendix C.

- Hydrogenated polydecene is an LT-UNK chemical when screened using Pharos, and therefore a full GreenScreen® is required.
- Hydrogenated polydecene is not listed on the U.S. DOT list.
- Hydrogenated polydecene is on the following lists for multiple endpoints. Specified lists for single endpoints are reported in individual hazard endpoints in the hazard assessment section below.
    - EC – CEPA DSL - Inherently Toxic to Humans (iTH)
    - EC – CEPA DSL – Inherently Toxic in the Environment (iTE)
    - German FEA - Substances Hazardous to Waters - Class 1 - Low Hazard to Waters

Hazard Statement and Occupational Control

Hydrogenated polydecene does not have any harmonized hazard statements, but is classified in its REACH dossier to GHS Category 1 for aspiration hazard with a hazard statement of H304: May be fatal if swallowed and enters airways, as indicated in Table 1. General personal protective equipment (PPE) recommendations are presented in Table 2, below. No occupational exposure limits (OELs) were identified.

[8] DOT lists are not required lists for GreenScreen® List Translator v1.4. They are reference lists only.

Table 1: GHS H Statements for Hydrogenated Polydecene (CAS #68037-01-4) (ECHA CHEM, CAS #68037-01-4, 2025)	
H Statement	**H Statement Details**
H304	Aspiration Hazard

Table 2: Occupational Exposure Limits and Recommended Personal Protective Equipment for Hydrogenated Polydecene (CAS #68037-01-4)			
Personal Protective Equipment (PPE)	**Reference**	**Occupational Exposure Limits (OEL)**	**Reference**
Safet glasses, goggles, face shield, gloves, protective clothing, respiratory protection	MakingCosmetics 2017	None	N/A

Physicochemical Properties of Hydrogenated Polydecene

Hydrogenated polydecene is a colorless and viscous liquid at room temperature. It is not soluble in water and its measured log K_{ow} of > 6.5 indicates it has a potential to bioaccumulate or is not bioavailable, depending on how high the value is. The vapor pressure for hydrogenated polydecene indicates that it is unlikely to volatilize.

Table 3: Physical and Chemical Properties of Hydrogenated Polydecene (CAS #68037-01-4)		
Property	**Value**	**Reference**
Molecular formula	UVCB	
SMILES Notation	UVCB	
Molecular weight	367-596	CIR 2020
Physical state	Liquid	EFSA 2020
Appearance	Colorless, odorless, viscous liquid	EFSA 2020
Melting point	<-57°C (ASTM D97)	ECHA, CAS #68037-01-4, 2025
Boiling point	217-419°C (ASTM D2887)	ECHA, CAS #68037-01-4, 2025
Vapor pressure	<0.545 Pa at 20°C (ASTM E1194-87)	ECHA, CAS #68037-01-4, 2025
Water solubility	<0.1 mg/L at 20°C (OECD Guideline 105)	ECHA, CAS #68037-01-4, 2025
Dissociation constant	N/A	
Density/specific gravity	0.82-0.83 g/mL at 15°C (ASTM D1298 / D4052)	ECHA, CAS #68037-01-4, 2025
Partition coefficient	Log K_{ow} > 6.5 at 20°C (OECD Guideline 117)	ECHA, CAS #68037-01-4, 2025

Toxicokinetics

The oral absorption of alkanes decreases with increasing carbon chain lengths. Absorption of n-alkanes with > 35 carbons were negligible, and branched alkanes have lower absorption than n-alkanes. The toxicokinetics of hydrogenated polydecene was studied in male Fischer rats. 1) Radiolabeled hydrogenated polydecene was administered to male Fischer rats (33/group) at single oral doses of 0, 30, 210, or 1,500 mg/animal and the radioactivity was measured in plasma, fat, kidney, liver, lymph node, spleen, gut wall, intestinal contents, urine, feces, carcass, skin and fur for 168 hours after exposure; 2) three rats received 30 mg/animal by intravenous injection and radioactivity was measured in plasma

after 168 hours; 3) three rats received an oral dose of 210 mg/animal daily for 14 days of the unlabeled test substance, followed by a single oral dose of radiolabeled test substance to study repeated dosing impact; and 4) three rats with cannulated bile ducts were exposed to a single oral dose of 210 mg/rat to study biliary, urinary and fecal excretion. Hydrogenated polydecene is poorly absorbed from the gastrointestinal tract following oral administration and is mainly excreted in the feces after single and repeated exposures (70% in the feces, 0.16% in the urine, and 0.01% in the bile after 48 hours, and 93-102% in the feces and < 1% in the urine after 168 hours) (EFSA 2020).

Hazard Classification Summary

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): L
Hydrogenated polydecene was assigned a score of Low for carcinogenicity based on negative results in a 2-year dermal carcinogenicity study in rats and supported by mostly negative modeled results from rule-based (VEGA IRFMN-Antares carcinogenicity model) and statistical-based models (Danish QSAR). GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is high based on measured data for the target chemical with support from modeled data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2010
  - Hydrogenated polydecene did not increase the incidence of tumors in male C3H mice (50/group) when applied to the skin twice a week for 104 weeks. Positive and negative control groups were reported as valid.
- Using the SMILES string of the hydrogenated 1-decene trimer that can be used as a conservative representative structure of hydrogenated polydecene, ToxServices performed modeling to support the evaluation of its carcinogenicity.
  - VEGA 2024
    - ToxServices modeled the carcinogenicity using the following VEGA carcinogenicity models: CAESAR, ISS, IRFMN-ISSCAN-CGX, IRFMN-Antares, IRFMN oral classification, and IRFMN inhalation classification. If an external compound is beyond the defined scope of a given model, it is considered outside that model's applicability domain (AD) and cannot be associated with a reliable prediction (Sahigara 2007). Values for AD index (ADI) range from 0 (worst case) to 1 (best case). Generally, ADI values of > 0.70 indicate that the prediction has moderate or better predictivity (Gad 2016). The following results with ADI values > 0.7 are produced:
    - The IRFMN-Antares carcinogenicity model predicts the compound to be a possible non-carcinogen, with an ADI of 0.785 (Appendix D).
  - U.S. EPA 2024b
    - The representative structure of hydrogenated polydecene cannot be evaluated using OncoLogic (Appendix E).
- DTU 2025
  - The CAS number of 68037-01-4 is found in the Danish QSAR database. The representative structure used in the database for this CAS is 1-decene. The in domain predictions are summarized below (Appendix F).

- Six of the seven databases of the E Ultra FDA RCA Cancer model predicted hydrogenated polydecene to be negative for carcinogenicity (male rate, female rat, rat, male mouse, mouse, and rodent), and the remaining database of the model predicted it to be positive for carcinogenicity (female mouse).
- Five of the seven databases of the Leadscope FDA RCA cancer model predicted hydrogenated polydecene to be negative for carcinogenicity (male rat, female rat, rat, mouse, rodent). The remaining predictions are out of domain.
- Hydrogenated polydecene does not contain ISS structural alerts for genotoxic or nongenotoxic carcinogenicity.
- The liver specific cancer in rat or mouse model battery predicted hydrogenated polydecene to be negative for carcinogenicity, based on negative and in domain predictions from CASE Ultra, Leadscope, and SciQSAR models.

Mutagenicity/Genotoxicity (M) Score (H, M, or L): L

Hydrogenated polydecene was assigned a score of Low for mutagenicity/genotoxicity based on negative mutagenicity results in *in vitro* assays and negative clastogenicity results in an *in vivo* study in rats. GreenScreen® criteria classify chemicals as a Low hazard for mutagenicity/genotoxicity when negative data are available for both gene mutations and chromosome aberrations, and they are not GHS classified (CPA 2018b). The confidence in the score is high based on reliable measured data for the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025
  - *In vitro:* Hydrogenated polydecene was negative for mutagenicity in a GLP-compliant bacterial reverse mutation assay conducted according to OECD Guideline 471in *Salmonella typhimurium* strains TA1535, TA1537, TA 98, and TA 100 at concentrations of 156.25, 312.5, 625, 1250, 2500, or 5000 µg/plate with and without metabolic activation. Vehicle and positive controls were reported as valid (Klimisch 1, reliable without restriction).
  - *In vitro:* Hydrogenated polydecene was negative for mutagenicity in a GLP-compliant bacterial reverse mutation assay similar to OECD Guideline 471 in *S. typhimurium* strains TA1535, TA1537, TA98, and TA100 at concentrations of 0, 0.10, 0.33, 1.00, 3.33, or 10.0 mg/plate with and without metabolic activation. Vehicle and positive controls were reported as valid (Klimisch 1, reliable without restriction).
- U.S. EPA 2010
  - *In vivo:* Hydrogenated polydecene has been tested in a mouse micronucleus assay using rats (15/sex/group; strain not specified). The test substance was administered via the dermal route at doses of 0, 800 or 2,000 mg/kg/day, 5 days/week for 13 weeks. At the end of the 13-week period, tissues were harvested for micronucleus evaluation. Femurs were taken from five rats/sex/dose and peripheral blood smears were made. No increase in micronucleus induction was observed in the groups administered the test substance at any of the harvest times when compared to the controls.

Reproductive Toxicity (R) Score (H, M, or L): L

Hydrogenated polydecene was assigned a score of Low for reproductive toxicity based on a lack of reproductive effects in a one generation reproductive study in rats. GreenScreen® criteria classify chemicals as a Low hazard for reproductive toxicity when adequate negative data are available and they

are not GHS classified (CPA 2018b). The confidence in the score is high based on reliable measured data for the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025, U.S. EPA 2010
  - In a GLP-compliant combined repeated-dose/reproductive toxicity test similar to OECD Guideline 415, Sprague-Dawley rats (30/sex/dose for F0 and 20/sex/dose for F1) were administered hydrogenated polydecene (composition: C30=31.27%; C40=45.02%; C50=17.44%; C60=6.27%) in polyethylene glycol via gavage at 0, 100, 500, or 1,000 mg/kg/day. Males were dosed for 4 weeks prior to mating and through the 15-day mating period and females were dosed from 4 weeks prior to mating, through pregnancy and until day 20 post-partum. Offspring were dosed for 91 days starting on day 22 post-partum. No treatment-related effects were reported on any of the reproductive parameters and the study authors identified a reproductive NOAEL of 1,000 mg/kg/day (Klimisch 1, reliable without restriction).

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): L

Hydrogenated polydecene was assigned a score of Low for developmental toxicity based on a lack of developmental effects in a one generation oral reproductive toxicity study, and a dermal prenatal developmental toxicity study in rats. GreenScreen® criteria classify chemicals as a Low hazard for developmental toxicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is high based on reliable measured data for the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025, U.S. EPA 2010
  - In the previously described GLP-compliant combined repeated-dose/reproductive toxicity test similar to OECD Guideline 415, Sprague-Dawley rats (30/sex/dose for F0 and 20/sex/dose for F1) were administered hydrogenated polydecene (composition: C30=31.27%; C40=45.02%; C50=17.44%; C60=6.27%) in polyethylene glycol via gavage at 0, 100, 500, or 1,000 mg/kg/day. Males were dosed for 4 weeks prior to mating and through the 15-day mating period and females were dosed from 4 weeks prior to mating, through pregnancy and until day 20 post-partum. Offspring were dosed for 91 days starting on day 22 post-partum. No treatment-related effects were reported on offspring survival, implantation loss, pup body weight, or sex ratio, and the study authors identified a developmental NOAEL of 1,000 mg/kg/day (Klimisch 1, reliable without restriction).
- U.S. EPA 2010
  - In a prenatal developmental toxicity study, pregnant Sprague-Dawley rats (15/dose) were dermally administered hydrogenated polydecene at 0, 800, or 2,000 mg/kg/day from gestation days 0 to 19. There was at most minimal dermal irritation at the site of application. There were no treatment related effects on food consumption of the dams. High dose dams had lower body weight gain on gestation days 13-16, but the statistical significance was not reported, and the overall weight gain during gestation was not significantly affected. Treated animals had changes in serum triglycerides and albumin levels but the statistical significance was not reported. There were no noticeable findings at necropsy. Pup survival, body weight, and crown-rump lengths were not affected, and there was no increase in

external, visceral, or skeletal malformations. Therefore, the NOAEL for maternal and developmental toxicities was 2,000 mg/kg/day, the highest dose tested.

Endocrine Activity (E) Score (H, M, or L): DG
Hydrogenated polydecene was assigned a score of Data Gap for endocrine activity based on the lack of data identified.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- No data were identified.

Group II and II* Human Health Effects (Group II and II* Human)

Note: Group II and Group II* endpoints are distinguished in the v 1.4 Benchmark system (the asterisk indicates repeated exposure). For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints. See GreenScreen® Guidance v1.4, Annex 2 for more details.

Acute Mammalian Toxicity (AT) (Group II) Score (vH, H, M, or L): L
Hydrogenated polydecene was assigned a score of Low for acute toxicity based on an oral LD_{50} value greater than 2,000 mg/kg in rats and an aerosol inhalation LC_{50} value greater than 5 mg/L/4h in rats. GreenScreen® criteria classify chemicals as a Low hazard for acute toxicity when adequate data are available and GHS classification is not warranted (CPA 2018b). The confidence in the score is high based on reliable measured data for the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025
  - *Oral*: LD_{50} (Sprague-Dawley rat) > 5,000 mg/kg (GLP, similar to OECD Guideline 420/423) (Klimisch 1, reliable without restriction).
  - *Inhalation*: LC_{50} (Sprague-Dawley rat) > 5.2 mg/L/4h (aerosol) (GLP, OECD Guideline 403) (Klimisch 1, reliable without restriction).
- U.S. EPA 2010
  - *Inhalation*: LC_{50} (Sprague-Dawley rat) > 2.5 mg/L/4h.

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-single) (Group II) Score (vH, H, M, or L): H
Hydrogenated polydecene was assigned a score of Low for systemic toxicity (single dose) based on a lack of specific target organ effects in rats administered a single oral dose of hydrogenated polydecene of 5,000 mg/kg and a single aerosol inhalation concentration of hydrogenated polydecene of 5.2 mg/L/4h. Hydrogenated polydecene is self-classified to aspiration hazard GHS Category 1 with the Hazard Statement of H304 "May be fatal if swallowed and enters airways" by its ECHA registration dossier authors. This is based on measured kinematic viscosity of some batches being less than 20 mm^2/s at 40°C and therefore, ToxServices conservatively classified it to GHS Category 1 for aspiration hazard. GreenScreen® criteria classify chemicals as a High hazard for systemic toxicity (single dose) when they are classified to GHS Category 1 for aspiration hazard (CPA 2018b). The confidence in the score is high based on reliable measured data for the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.

- ECHA, CAS #68037-01-4, 2025
    - *Oral*: In a GLP-compliant acute oral toxicity study similar to OECD Guideline 423 and 420, Sprague-Dawley rats (5/sex) were administered a gavage dose of 5,000 mg/kg hydrogenated polydecene and observed for 14 days. No mortalities occurred and no significant gross pathology was observed. Clinical signs included transient mild depression and oily hair coats (Klimisch 1, reliable without restriction).
    - *Inhalation*: In a GLP-compliant OECD Guideline 403 acute inhalation toxicity study, Sprague-Dawley rats (6/sex) were administered a nose only aerosol concentration of 5.2 mg/L hydrogenated polydecene for 4 hours and observed for 14 days. No mortalities occurred, there was no significant change in body weight, and no gross pathology abnormality was observed. Clinical signs included labored breathing (Klimisch 1, reliable without restriction). *ToxServices did not consider labored breathing sufficient as evidence of respiratory tract irritation (GHS Category 3) based on the lack of findings during necropsy or other clinical signs of irritation.*
    - Hydrogenated polydecene has a kinematic viscosity of 47.5 mm^2/s at 40°C in an ASTM 445 study (Klimisch 2, reliable with restrictions).
        - *This would not warrant GHS classification based on a kinematic viscosity greater than 20 mm^2/s at 40°C (UN 2023).*
    - Hydrogenated polydecene has a kinematic viscosity of 31 mm^2/s at 40°C in an ASTM D445 study (Klimisch 2, reliable with restrictions).
        - *This would not warrant GHS classification based on a kinematic viscosity greater than 20 mm^2/s at 40°C (UN 2023).*
    - Hydrogenated polydecene has a kinematic viscosity of 17.8-46.5 mm^2/s at 40°C in an ASTM D445 study (Klimisch 2, reliable with restrictions).
        - *This would warrant GHS classification based on kinematic viscosity potentially less than 20 mm^2/s at 40°C (UN 2023).*

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-repeat) (Group II*) Score (H, M, or L): L

Hydrogenated polydecene was assigned a score of Low for systemic toxicity (repeated dose) based on a lack of specific target organ effects in rats administered repeated oral doses of hydrogenated polydecene greater than 100 mg/kg in subchronic oral studies. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (repeated dose) when adequate data are available and GHS classification is not warranted (CPA 2018b). The confidence in the score is high based on reliable measured data for the target chemical.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025
    - *Oral:* In a GLP-compliant subchronic oral toxicity study similar to OECD Guideline 407, Fischer 344 rats (5/sex/dose) were provided 0, 8,000, 20,000, or 50,000 ppm (1,039, 2,538, or 6,245 mg/kg/day for males and 995, 2481, or 6771 mg/kg/day for females according to the ECHA CHEM dossier) hydrogenated polydecene (purity not reported) in feed for 29 days. No effects on clinical signs, body weight, food efficiency, organ weights, gross pathology, or histopathology were reported. Authors of the ECHA CHEM dossier identified a NOAEL of 50,000 ppm (6,245 mg/kg/day for males and 6,771 mg/kg/day for females) (Klimisch 2, reliable with restrictions).

- *Oral:* In a GLP-compliant subchronic oral toxicity study similar to OECD Guideline 408, Sprague-Dawley rats (20/sex/dose) were administered 0, 100, 500, or 1,000 mg/kg/day hydrogenated polydecene (composition: C30=31.27%; C40=45.02%; C50=17.44%; C60=6.27%) via gavage for 91 days. No effects on clinical signs, body weight, ophthalmoscopic examination, hematology, clinical chemistry, urinalysis, organ weights, gross pathology, or histopathology were reported. Authors of the ECHA CHEM dossier identified a NOAEL of 1,000 mg/kg/day (Klimisch 1, reliable without restriction).
- *Oral:* In a GLP-compliant subchronic oral toxicity study according to OECD Guideline 408, Fischer 344 rats (10/sex/dose) were provided 0, 1,000, 7,000, or 50,000 ppm hydrogenated polydecene (composition: 52.98% C40; 27.81% C30; 14.28% C50; 4.25% C60; 0.60% C20; 0.08% C10-C20) in feed for 13 weeks (equivalent to 77.5, 553.7, and 4,159.4 mg/kg/day for males and 85.5, 611.5, and 4,619.9 mg/kg/day for females according to the ECHA CHEM dossier). The only clinical signs observed were oily and ungroomed coats, soft feces, and staining in the high dose group. No effects on body weight, food efficiency, ophthalmoscopic examination, clinical chemistry, urinalysis, gross pathology, or histopathology were reported. Absolute and relative liver weights in males increased slightly and dose dependently, but were comparable to controls after a 4-week recovery period. Erythrocyte counts, hemoglobin, and packed cell volume were slightly increased at the two highest doses and platelet counts were slightly increased at the high dose. These changes were not apparent after the recovery period, and no changes were noted in bone marrow smears. The authors of the ECHA CHEM dossier did not consider the changes in hematology parameters and liver weight toxicologically significant, and identified a NOAEL of 50,000 ppm (2,149.4 mg/kg/day for males and 4,619.9 mg/kg/day for females) (Klimisch 1, reliable without restriction).

- U.S. EPA 2010
  - In a range-finding study, female Sprague-Dawley rats (5/dose) were exposed to hydrogenated polydecene by gavage at 0, 500, 2,500, or 5,000 mg/kg/day, 5 days per week, for 4 weeks. There were no deaths or body weight changes related to treatment. Clinical signs attributable to treatment included oily staining round the anus and soft stool. Gross pathological findings were unremarkable, and there were no histopathological abnormalities in the liver. U.S. EPA assigned a NOAEL of 5,000 mg/kg/day, the highest dose tested.
  - There were no mortalities, clinical signs of toxicity, effects on body weight or organ weight, and no histopathological changes in Sprague-Dawley rats (20/sex/dose) provided hydrogenated polydecene in the feed at 0, 500, 5,000, or 20,000 ppm (equivalent to 0, 25, 250, or 1,000 mg/kg/day according to U.S. EPA) for 90 days. A dose-dependent increase in serum albumin/globulin ratio in males and phosphorus levels in females were measured, but these effects were not considered adverse. The study authors assigned a NOAEL of 1,000 mg/kg/day, the highest dose tested.
  - There were no treatment-related mortalities, clinical signs of toxicity, effects on body weight, organ weight, ophthalmology, or hematology in Fischer 344 rats (10/sex/dose) provided hydrogenated polydecene in the feed at 0, 200, or 20,000 ppm (equivalent to 0, 10, or 1,000 mg/kg/day according to U.S. EPA) for 90 days. A statistically significant change in serum levels were observed, but these effects were not considered adverse. The study authors assigned a NOAEL of 1,000 mg/kg/day, the highest dose tested.

Neurotoxicity (single dose, N-single) (Group II) Score (vH, H, M, or L): *L*
Hydrogenated polydecene was assigned a score of Low for neurotoxicity (single dose) based a lack of neurotoxic effects in rats administered a single oral dose of hydrogenated polydecene at 5,000 mg/kg

and a single aerosol inhalation concentration of hydrogenated polydecene at 5.2 mg/L/4h. GreenScreen® criteria classify chemicals as a Low hazard for neurotoxicity (single dose) when adequate data are available and GHS classification is not warranted (CPA 2018b). The confidence in the score is low as there were no specific neurotoxicity examinations.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025
  - *Oral*: In a GLP-compliant acute oral toxicity study similar to OECD Guideline 423 and 420, Sprague-Dawley rats (5/sex) were administered a gavage dose of 5,000 mg/kg hydrogenated polydecene and observed for 14 days. No mortalities occurred and no significant gross pathology was observed. Clinical signs included transient mild depression and oily hair coats (Klimisch 1, reliable without restriction).
  - *Inhalation*: In a GLP-compliant OECD Guideline 403 acute inhalation toxicity study, Sprague-Dawley rats (6/sex) were administered a nose only aerosol concentration of 5.2 mg/L hydrogenated polydecene for 4 hours and observed for 14 days. No mortalities occurred, and no gross pathology abnormality was observed. Clinical signs included labored breathing (Klimisch 1, reliable without restriction).

Neurotoxicity (repeated dose, N-repeated) (Group II*) Score (H, M, or L): L

Hydrogenated polydecene was assigned a score of Low for neurotoxicity (repeated dose) based on a lack of neurotoxic effects in rats administered repeated oral doses of surrogate 1-dodecene trimer, hydrogenated greater than 100 mg/kg in a subchronic study. GreenScreen® criteria classify chemicals as a Low hazard for neurotoxicity (repeated dose) when adequate data are available and GHS classification is not warranted (CPA 2018b). The confidence in the score is high based on reliable measured data for a strong surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025
  - *Oral: Surrogate: 1-Dodecene trimer, hydrogenated (CAS #151006-62-1):* In a GLP-compliant subchronic oral toxicity study conducted according to OECD Guideline 408, Sprague-Dawley rats (10/sex/dose) were administered test substance at doses of 0, 50, 250, or 1,000 mg/kg/day via gavage for 90 days. Animals were evaluated for neurobehavior in a battery of functional tests: sensory activity, grip strength, and motor activity. There were no adverse effects on any parameters compared to controls for the treated animals (Klimisch 1, reliable without restriction). *ToxServices assigned a NOAEL of 1,000 mg/kg/day, the highest dose tested, for neurotoxicity.*

Skin Sensitization (SnS) (Group II*) Score (H, M, or L): L

Hydrogenated polydecene was assigned a score of Low for skin sensitization based on a less than 30% population response in guinea pig maximization tests. GreenScreen® criteria classify chemicals as a Low hazard for skin sensitization when adequate data are available and GHS classification is not warranted (CPA 2018b). The confidence in the score is high based on reliable measured data for the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.

- ECHA, CAS #68037-01-4, 2025
    - Hydrogenated polydecene was not sensitizing in a GLP-compliant guinea pig maximization test similar to OECD Guideline 406 with Hartley guinea pigs (10/sex) induced with 5% test substance in mineral oil under occlusive epicutaneous conditions and challenged at 10% test article. No sensitization responses were seen in any animal (Klimisch 1, reliable without restriction).
    - Hydrogenated polydecene was not sensitizing in a GLP-compliant guinea pig maximization test conducted according to OECD Guideline 406 with female Hartley guinea pigs (n=20) intradermally and topically induced and challenged with 100% test compound. Intradermal induction was performed with 25% Freund's Complete Adjuvant. A positive response was seen in 2/10 animals in challenge, and in 1/10 animals at rechallenge. The authors of the ECHA CHEM dossier concluded that hydrogenated polydecene was not sensitizing in this study (Klimisch 1, reliable without restriction).
        - *Based on the less than 30% population response, GHS Category 1 classification is not warranted.*

Respiratory Sensitization (SnR) (Group II*) Score (H, M, or L): *L*

Hydrogenated polydecene was assigned a score of Low for respiratory sensitization based on the lack of dermal sensitization potential according to the ECHA guidance (2017). GreenScreen® criteria classify chemicals as a Low hazard for respiratory sensitization when they are not GHS classified (CPA 2018b). Confidence in the score is low as this evaluation does not include non-immunologic mechanisms of respiratory sensitization, and no specific data are available for respiratory sensitization.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- Based on the weight of evidence and guidance from ECHA regarding assessment of respiratory sensitization potential, a score of Low was assigned. The guidance from ECHA states that the mechanisms leading to respiratory sensitization are essentially similar to those leading to skin sensitization (ECHA 2017). ECHA recommended that if a chemical is not a dermal sensitizer based on high quality data, it is unlikely to be a respiratory sensitizer. ECHA also noted that this rationale does not cover respiratory hypersensitivity caused by non-immunological mechanisms, for which human experience is the main evidence of activity (ECHA 2017). As hydrogenated polydecene was not sensitizing to the skin (see skin sensitization section above), and a literature search did not find any human evidence of respiratory sensitization by hydrogenated polydecene, hydrogenated polydecene is not expected to be a respiratory sensitizer.

Skin Irritation/Corrosivity (IrS) (Group II) Score (vH, H, M, or L): L

Hydrogenated polydecene was assigned a score of Low for skin irritation/corrosivity based on negative results in two dermal irritation studies with rabbits. GreenScreen® criteria classify chemicals as a Low hazard for skin irritation/corrosivity when GHS classification is not warranted (CPA 2018b). The confidence in the score is high based on measured data for the target chemical.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025
    - In a GLP-compliant skin irritation study similar to OECD Guideline 404, female New-Zealand White rabbits (n=6) were treated with 0.5 mL of undiluted hydrogenated polydecene on both intact and abraded skin for 24 hours under occlusive conditions.

Animals were observed for 3 days. Treatment caused very slight to well-defined erythema on both intact and abraded sites (mean scores 0.67-0.75) and slight edema at 3 intact and 1 abraded site at the end of treatment (mean scores 0.08-0.25). The effects were partially reversible within 72 hours. The primary irritation index (PII) was determined to be 0.9. Individual animal scores were not provided. Based on the results of the study, the authors of the ECHA CHEM dossier concluded that hydrogenated polydecene was not irritating to the skin in this study (Klimisch 2, reliable with restrictions).

- In another GLP-compliant skin irritation study similar to OECD Guideline 404, New-Zealand White rabbits (3/sex) were treated with 0.5 mL of undiluted hydrogenated polydecene on both intact and abraded skin for 24 hours under occlusive conditions. Animals were observed for 3 days. Treatment caused mild erythema on both intact and abraded sites (mean score 0.42) and mild edema at abraded sites at the end of treatment (mean score 0.08). The effects were fully reversible within 72 hours. The PII was determined to be 0.5. Individual animal scores were not provided. Based on the results of the study, the authors of the ECHA CHEM dossier concluded that hydrogenated polydecene was not irritating to the skin in this study (Klimisch 2, reliable with restrictions).

Eye Irritation/Corrosivity (IrE) (Group II) Score (vH, H, M, or L): L

Hydrogenated polydecene was assigned a score of Low for eye irritation/corrosivity based on negative results in two eye irritation studies with rabbits. GreenScreen® criteria classify chemicals as a Low hazard for eye irritation/corrosivity when GHS classification is not warranted (CPA 2018b). The confidence in the score is high based on measured data for the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025
  - In a GLP-compliant ocular irritation test similar to OECD Guideline 405, New Zealand White rabbits (3/sex) were administered ocular instillations of 0.1 mL undiluted hydrogenated polydecene and were observed for 3 days. Conjunctival changes were observed in 5 of the 6 rabbits. At 24, 48, and 72 hours, the mean conjunctival scores were 1, 1, 0, 0.67, 0.33, and 0.67. At 24, 48, and 72 hours, the mean chemosis scores were 0.33, 0, 0, 0.33, 0, and 1. At 24, 48, and 72 hours, the mean corneal opacity and mean iris scores were 0 for all animals. The authors of the ECHA CHEM dossier concluded that the test substance was not irritating to the eyes in this study (Klimisch 1, reliable without restriction).
    - *Based on the individual animals scores provided, GHS classification is not warranted.*
  - In another GLP-compliant ocular irritation test similar to OECD Guideline 405, New-Zealand White rabbits (3/sex) were instilled with 0.1 mL of hydrogenated polydecene in the right eye and the test material was allowed to remain in the eye without rinsing. An observation period of 3 days followed. Treatment caused slight conjunctival erythema at 24 hours in 4 animals with effects being fully reversible in one animal. The overall irritation index was determined to be 1.67/110 at 72 hours. Individual animals scores were not provided. Based on the results of the study, the authors of the ECHA CHEM dossier concluded that hydrogenated polydecene was not irritating to the eye in this study (Klimisch 1, reliable without restriction).

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): L
Hydrogenated polydecene was assigned a score of Low for acute aquatic toxicity based on L/EC_{50} values >100 mg/L in fish, daphnid, and algae. GreenScreen® criteria classify chemicals as a Low hazard for acute aquatic toxicity when L/EC_{50} values are greater than 100 mg/L in fish, daphnid, and algae (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for all three trophic levels.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025
  - 96-hour LC_{50} (*Oncorhynchus mykiss*, fish) > 1,000 mg/L as water accommodated fractions (WAFs) (GLP, EPA-660/3-75-009) (Klimisch 1, reliable without restriction).
  - 96-hour LC_{50} (*O. mykiss*, fish) > 1,000 mg/L as WAFs (GLP, OECD Guideline 203) (Klimisch 1, reliable without restriction).
  - 48-hour mobility EC_{50} (*Daphnia magna,* Daphnia) > 1,000 mg/L as WAF (GLP, OECD Guideline 202) (Klimisch 1, reliable without restriction).
  - 48-hour mobility EC_{50} (*D. magna,* Daphnia) > 130 mg/L as WAF (GLP) (Klimisch 2, reliable with restrictions).
  - 72-hour EC_{50} (*Scenedesmus capricornutum,* algae) > 1,000 mg/L as WAF for biomass and growth rate (GLP, OECD Guideline 201) (Klimisch 2, reliable with restrictions).

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): *L*
Hydrogenated polydecene was assigned a score of Low for chronic aquatic toxicity based on an experimental 21-day reproduction NOEC of 125 mg/L for Daphnid and an experimental 72-hour biomass / growth rate NOEC of > 1,000 mg/L in algae. GreenScreen® criteria classify chemicals as a Low hazard for chronic aquatic toxicity when chronic values are greater than 10 mg/L (CPA 2018b). The confidence in the score is low as data were not identified for the fish trophic level.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025
  - 21-day NOEC (*D. magna,* Daphnia) = 125 mg/L as WAF based on mortality, timing of first brood, number of offspring, length and weight (GLP, OECD Guideline 211) (Klimisch 1, reliable without restriction).
  - 72-hour NOEC (*S. capricornutum,* algae) > 1,000 mg/L as WAF for biomass and growth rate (GLP, OECD Guideline 201) (Klimisch 2, reliable with restrictions).

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): *H*
Hydrogenated polydecene was assigned a score of High for persistence based on an estimated half-life of 135 days in the major compartment, sediment, for the longest constituent hydrogenated 1-decene hexamer. GreenScreen® criteria classify chemicals as a High hazard for persistence when soil and sediment are the dominant environmental compartment with a half-life 60-180 days (CPA 2018b). The confidence in the score is low based on modeled data.

- Authoritative and Screening Lists

  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* EC – CEPA DSL – Persistent.
- ECHA, CAS #68037-01-4, 2025
  - Hydrogenated polydecene was not readily biodegradable in biodegradation assay conducted according to OECD Guideline 301D (Ready Biodegradability: Closed Bottle Test). In this assay, aerobic activated sludge was exposed to the test substance (100% purity) at 2 mg/L for 28 days. A biodegradation rate of 2% was achieved at the end of the exposure period (Klimisch 1, reliable without restriction).
- U.S. EPA 2017
  - Using the representative longest constituent of hydrogenated polydecene, hydrogenated 1-decene hexamer, the following prediction results were obtained:
  - BIOWIN modeling predicts that the substance is not readily biodegradable. Level II Fugacity modeling (EQC default) predicts 66.6% will partition to sediment with a half-life of 135 days, 29.7% to soil with a half-life of 30 days, and 3.65% to water with a half-life of 15 days (Appendix G).
- Based on the weight of evidence, a score of High is assigned for hydrogenated polydecene. It is listed as persistent by Environment Canada (EC) (equivalent to a GreenScreen® score of High or Very High), which is supported by measured data demonstrating it is not readily biodegradable in a ready biodegradability test conducted according to OECD Guideline 301D. No partitioning data are identified, and EPI Suite™ modeling predicts a half-life of 135 days in its major compartment, sediment, for the longest constituent. This corresponds to a High score.

Bioaccumulation (B) Score (vH, H, M, L, or vL): *vL*
Hydrogenated polydecene was assigned a score of Very Low for bioaccumulation based on an modeled BAF values of < 100 for the shortest and longest constituents. GreenScreen® criteria classify chemicals as a Low hazard for bioaccumulation when BCF or BAF values are less than or equal to 100 (CPA 2018b). The confidence in the score is low based on the reliance on modeled data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2017
  - For the smallest constituent of hydrogenated polydecene, the hydrogenated trimer of 1-decene, BCFBAF predicts a BAF of 4.797 using the Arnot-Gobas method for the upper trophic level, based on an estimated log K_{ow} of 14.93 (Appendix H).
  - For the longest constituent of hydrogenated polydecene, the hydrogenated hexamer of 1-decene, BCFBAF predicts a BAF of 0.893 using the Arnot-Gobas method for the upper trophic level, based on an estimated log K_{ow} of 29.44 (Appendix G).

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): *L*
Hydrogenated polydecene was assigned a score of Low for reactivity based on the lack of structural alerts for oxidizing and explosive properties. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when it does not warrant GHS classification for any of the reactivity sub-endpoints and the chemical is not present on authoritative or screening lists (CPA 2018b). The confidence in the score is low based on the lack of measured data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.

  - *Screening:* Not present on any screening lists for this endpoint.
- No measured data were identified. Therefore, screening procedures for explosivity were used here to estimate the reactivity property of hydrogenated polydecene. These procedures are listed in the GHS (UN 2023).
  - Based on the structure of its components or moieties, hydrogenated polydecene is not considered explosive or self-reactive due to lack of functional groups associated with explosive or self-reactive properties (See Appendix I).
  - Based on the structure of its components or moieties, hydrogenated polydecene is not considered to have oxidizing properties as it does not contain any structural groups known to be correlated with a tendency to react exothermally with combustible materials. Specifically, organic substances which contain oxygen, fluorine, or chlorine where these elements are chemically bonded only to carbon or hydrogen, classification as an oxidizing liquid need not be applied. Therefore, as the molecular structure of hydrogenated polydecene has no oxygens, it is not expected to be oxidizing.
- MakingCosmetics 2017
  - A safety data sheet for hydrogenated polydecene states that it has a reactivity hazard of 0 from NFPA ("Normally stable, even under fire exposure conditions, and is not reactive with water") (NFPA 2017).

Flammability (F) Score (vH, H, M, or L): L

Hydrogenated polydecene was assigned a score of Low for flammability based on having a measured flash point of 219-257°C, which is above the guidance value of 93°C for GHS Category 4 for flammable liquids. GreenScreen® criteria classify chemicals as a Low hazard for flammability when GHS classification is not warranted (CPA 2018b). The confidence in the score is high based on measured data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #68037-01-4, 2025
  - Hydrogenated polydecene has a measured flash point of 219-257°C obtained in a test conducted according to ASTM D92 (Klimisch 2, reliable with restrictions).
    - According to GHS criteria (UN 2023), the flash point of 219-257°C is above the guidance value of 93°C for Category 4 flammable liquid, therefore GHS classification is not warranted.
- MakingCosmetics 2017
  - A safety data sheet for hydrogenated polydecene states that it has a flammability hazard of 1 from NFPA ("Suggests that the material requires considerable preheating before it will ignite") (NFPA 2017).

Use of New Approach Methodologies (NAMs)[9] in the Assessment, Including Uncertainty Analyses of Input and Output

New Approach Methodologies (NAMs) used in this GreenScreen® include *in vitro* tests for genotoxicity, expert-based guidance on evaluating respiratory sensitization, and *in silico* modeling for carcinogenicity, persistence, and bioaccumulation. NAMs are non-animal alternatives that can be used alone or in combination to provide information for safety assessment (Madden et al. 2020). At present, there is not a uniformly accepted framework on how to report and apply individual NAMs (U.S. EPA 2020, OECD 2020). The expanded application of NAMs greatly amplifies the need to communicate uncertainties associated with their use. As defined by EFSA (2018), uncertainty is "a general term referring to all types of limitations in available knowledge that affect the range and probability of possible answers to an assessment question." The quality, utility, and accuracy of NAM predictions are greatly influenced by two primary types of uncertainties (OECD 2020):

- Type I: Uncertainties related to the input data used
- Type II: Uncertainties related to extrapolations made

As shown in Table 4, Type I (input data) uncertainties in hydrogenated polydecene's NAMs dataset include absence of/insufficient experimental data for carcinogenicity, respiratory sensitization, and bioaccumulation, and lack of established test methods for respiratory sensitization. Hydrogenated polydecene's Type II (extrapolation output) uncertainties include lack of defined applicability domains for the carcinogenicity structural alerts by ISS in the Danish QSAR database, limitations of *in vitro* genotoxicity assays to mimic *in vivo* metabolic conditions, and lack of consideration of non-immunological mechanisms of respiratory sensitization. Some of hydrogenated polydecene's type II uncertainties were alleviated by the use of *in vitro* test batteries and/or in combination of *in vivo* data.

Table 4: Summary of NAMs Used in the GreenScreen® Assessment, Including Uncertainty Analyses	
Uncertainty Analyses (OECD 2020)	
Type I Uncertainty: Data/Model Input	**Carcinogenicity:** Experimental data are available for only the dermal route, which has limited bioavailability. **Genotoxicity:** No Type I uncertainty is identified on using the *in vitro* genotoxicity assays as they are considered relevant (appropriate for the evaluation of the corresponding hazards as recommended in the OECD Guideline), reliable (they have Klimisch scoring of 2 or 1) and adequate (validated methods). **Respiratory sensitization**: No experimental data are available and there are no validated test methods. **Bioaccumulation:** No experimental data are available.
Type II Uncertainty: Extrapolation Output	**Carcinogenicity:** The ISS structural alerts for genotoxic and nongenotoxic carcinogenicity (in Danish QSAR database) do not have applicability domains. **Genotoxicity:** The bacterial reverse mutation assay (as defined in OECD Guideline 471) only tests point-mutation inducing activity in

[9] NAMs refers to any non-animal technology, methodology, approach, or combination thereof that inform chemical hazard and risk assessments. NAMs include *in silico*/computational tools, *in vitro* biological profiling (e.g., cell cultures, 2,3-D organotypic culture systems, genomics/transcriptomics, organs on a chip), and frameworks (i.e., adverse outcome pathways (AOPs), defined approaches (DA), integrated approaches to testing and assessment (IATA).

	non-mammalian cells, and the exogenous metabolic activation system does not entirely mimic *in vivo* conditions[10]. **Respiratory sensitization**: The ECHA guidance (2017) does not evaluate non-immunologic mechanisms for respiratory sensitization.	
Endpoint	**NAMs Data Available and Evaluated? (Y/N)**	**Types of NAMs Data (*in silico* modeling/*in vitro* biological profiling/frameworks)**
Carcinogenicity	Y	*In silico* modeling: VEGA / Danish QSAR database
Mutagenicity	Y	*In vitro* data: Bacterial reverse mutation assay
Reproductive toxicity	N	
Developmental toxicity	N	
Endocrine activity	N	
Acute mammalian toxicity	N	
Single exposure systemic toxicity	N	
Repeated exposure systemic toxicity	N	
Single exposure neurotoxicity	N	
Repeated exposure neurotoxicity	N	
Skin sensitization	N	
Respiratory sensitization	Y	ECHA guidance (2017)
Skin irritation	N	
Eye irritation	N	
Acute aquatic toxicity	N	
Chronic aquatic toxicity	N	
Persistence	Y	Non-animal testing: OECD Guideline 301 Biodegradation tests *In silico* modeling: EPI Suite™
Bioaccumulation	Y	*In silico* modeling: EPI Suite™

[10] https://www.oecd-ilibrary.org/docserver/9789264071247-en.pdf?expires=1614097593&id=id&accname=guest&checksum=89925F80B9F4BD2FFC6E90F94A0EE427

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APPENDIX A: Hazard Classification Acronyms
(in alphabetical order)

(AA) Acute Aquatic Toxicity

(AT) Acute Mammalian Toxicity

(B) Bioaccumulation

(C) Carcinogenicity

(CA) Chronic Aquatic Toxicity

(D) Developmental Toxicity

(E) Endocrine Activity

(F) Flammability

(IrE) Eye Irritation/Corrosivity

(IrS) Skin Irritation/Corrosivity

(M) Mutagenicity and Genotoxicity

(N) Neurotoxicity

(P) Persistence

(R) Reproductive Toxicity

(Rx) Reactivity

(SnS) Sensitization- Skin

(SnR) Sensitization- Respiratory

(ST) Systemic/Organ Toxicity

APPENDIX B: Results of Automated GreenScreen® Score Calculation for Hydrogenated Polydecene (CAS #68037-01-4)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

GREEN SCREEN FOR SAFER CHEMICALS

GreenScreen® Score Inspector

Table 1: Hazard Table

			Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
			Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
Table 2: Chemical Details									S	R *	S	R *	*	*								
Inorganic Chemical?	Chemical Name	CAS#	C	M	R	D	E	AT	STs	STr	Ns	Nr	SNS*	SNR*	IrS	IrE	AA	CA	P	B	Rx	F
No	Hydrogenated Polydecene	68037-01-4	L	L	L	L	DG	L	H	L	*L*	L	L	*L*	L	L	L	*L*	*H*	*vL*	*L*	L

Table 3: Hazard Summary Table

Benchmark	a	b	c	d	e	f	g
1	No	No	No	No	No		
2	No	No	Yes	No	No	No	No
3	STOP						
4	STOP						

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Hydrogenated Polydecene	2

Note: Chemical has not undergone a data gap assessment. Not a Final GreenScreen™ Score

Table 6

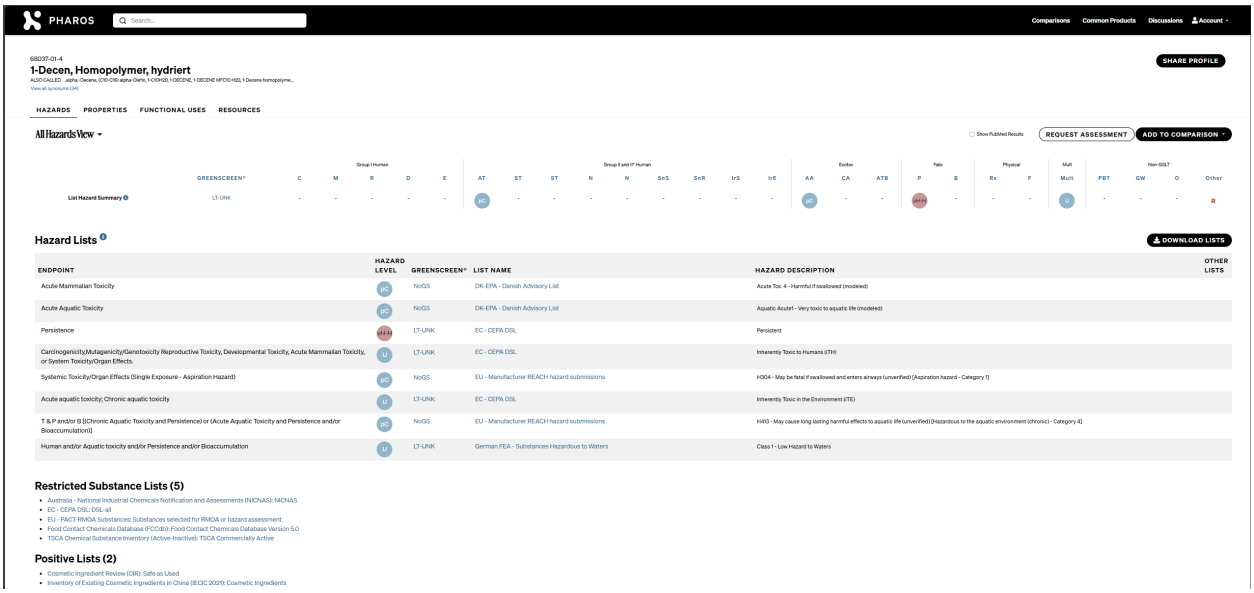
Chemical Name	Final GreenScreen® Benchmark Score
Hydrogenated Polydecene	2

After Data gap Assessment
Note: No Data gap Assessment Done if Preliminary GS Benchmark Score is 1.

Table 5: Data Gap Assessment Table

Datagap Criteria	a	b	c	d	e	f	g	h	i	j	bm4	End Result
1												
2	Yes	Yes	Yes	Yes	Yes							2
3												
4												

APPENDIX C: Pharos Output for Hydrogenated Polydecene (CAS #68037-01-4)



PHAROS

Comparisons Common Products Discussions Account

68037-01-4

1-Decen, Homopolymer, hydriert

ALSO CALLED: ...alpha.-Decene, (C10-C16)-alpha-Olefin, 1-C10H20, 1-DECENE, 1-DECENE MPC10-H20, 1-Decene homopolyme...

View all synonyms (34)

SHARE PROFILE

HAZARDS PROPERTIES FUNCTIONAL USES RESOURCES

All Hazards View

Show PubMed Results REQUEST ASSESSMENT ADD TO COMPARISON

		Group I Human					Group II and II* Human								Ecotox			Fate		Physical		Mult	Non-GILT			
	GREENSCREEN®	C	M	R	D	E	AT	ST	ST	N	N	SnS	SnR	IrS	IrE	AA	CA	ATB	P	B	Rx	F	Mult	PBT	GW	O	Other
List Hazard Summary	LT-UNK	-	-	-	-	-	vH	-	-	-	-	-	-	-	-	vH	-	-	vH	-	-	-	U	-	-	-	R

Hazard Lists

DOWNLOAD LISTS

ENDPOINT	HAZARD LEVEL	GREENSCREEN®	LIST NAME	HAZARD DESCRIPTION	OTHER LISTS
Acute Mammalian Toxicity	vH	NoGS	DK-EPA - Danish Advisory List	Acute Tox. 4 - Harmful if swallowed (modeled)	
Acute Aquatic Toxicity	vH	NoGS	DK-EPA - Danish Advisory List	Aquatic Acute1 - Very toxic to aquatic life (modeled)	
Persistence	vH-I-I	LT-UNK	EC - CEPA DSL	Persistent	
Carcinogenicity;Mutagenicity/Genotoxicity Reproductive Toxicity, Developmental Toxicity, Acute Mammalian Toxicity, or System Toxicity/Organ Effects.	U	LT-UNK	EC - CEPA DSL	Inherently Toxic to Humans (ITH)	
Systemic Toxicity/Organ Effects (Single Exposure - Aspiration Hazard)	vH	NoGS	EU - Manufacturer REACH hazard submissions	H304 - May be fatal if swallowed and enters airways (unverified) (Aspiration hazard - Category 1)	
Acute aquatic toxicity; Chronic aquatic toxicity	U	LT-UNK	EC - CEPA DSL	Inherently Toxic in the Environment (ITE)	
T & P and/or B [(Chronic Aquatic Toxicity and Persistence) or (Acute Aquatic Toxicity and Persistence and/or Bioaccumulation)]	vH	NoGS	EU - Manufacturer REACH hazard submissions	H413 - May cause long lasting harmful effects to aquatic life (unverified) (Hazardous to the aquatic environment (chronic) - Category 4)	
Human and/or Aquatic toxicity and/or Persistence and/or Bioaccumulation	U	LT-UNK	German FEA - Substances Hazardous to Waters	Class 1 - Low Hazard to Waters	

Restricted Substance Lists (5)

- Australia - National Industrial Chemicals Notification and Assessments (NICNAS): NICNAS
- EC - CEPA DSL: DSL-all
- EU - PACT-RMOA Substances: Substances selected for RMOA or hazard assessment
- Food Contact Chemicals Database (FCCdb): Food Contact Chemicals Database Version 5.0
- TSCA Chemical Substance Inventory (Active-Inactive): TSCA Commercially Active

Positive Lists (2)

- Cosmetic Ingredient Review (CIR): Safe as Used
- Inventory of Existing Cosmetic Ingredients in China (IECIC 2021): Cosmetic Ingredients

APPENDIX D: VEGA Carcinogenicity Modeling Results for Hydrogenated 1-Decene Trimer

1. Prediction Summary

Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC(CCCCCCCC)CC(C)CCCCCCCC
Experimental value: -
Predicted Carcinogen activity: Carcinogen
P(Carcinogen): 0.781
P(NON-Carcinogen): 0.219
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

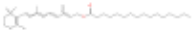
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 7235-40-7
Dataset id:130 (Training Set)
SMILES:
C(=CC=C(C=CC=C(C=CC1=C(C)CCCC1(C)C)C)C)C=C(C=CC=C(C=CC2=C(C)CCCC2(C)C)C)C
Similarity: 0.634
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

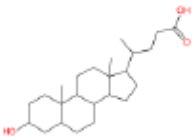
Compound #2

CAS: 35449-36-6
Dataset id:345 (Training Set)
SMILES: OCC(C)(C)CCCCCCC(C)(C)CO
Similarity: 0.611
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #3

CAS: 79-81-2
Dataset id:693 (Training Set)
SMILES: O=C(OCC=C(C=CC=C(C=CC1=C(C)CCCC1(C)C)C)C)CCCCCCCCCCCCCCCC
Similarity: 0.604
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

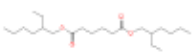


Compound #4

CAS: 434-13-9
Dataset id:413 (Training Set)
SMILES: O=C(O)CCC(C)C2CCC3C4CCC1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.602
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #5

CAS: 1643-20-5
Dataset id:273 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.597
Experimental value : NON-Carcinogen
Predicted value : Carcinogen



Compound #6

CAS: 103-23-1
Dataset id:315 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.597
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.622 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✖	Concordance for similar molecules Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✔	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✔	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..
✔	Model class assignment reliability Pos/Non-Pos difference = 0.562 Explanation: model class assignment is well defined..
✔	Neural map neurons concordance Neurons concordance = 1 Explanation: predicted value agrees with experimental values of training set compounds laying in the same neuron..

Symbols explanation:

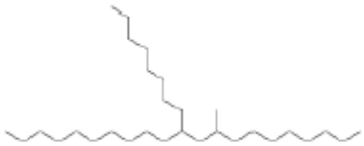
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0 -

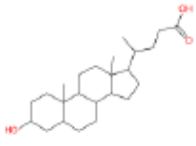


Prediction: Reliability:

Prediction is NON-Carcinogen, but the result shows some critical aspects, which require to be checked:
- No similar compounds with known experimental value in the training set have been found
- some similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC(CCCCCCCC)CC(C)CCCCCCCC
Experimental value: -
Predicted Carcinogen activity: NON-Carcinogen
Structural Alerts: -
Reliability: The predicted compound could be out of the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 434-13-9
Dataset id:117 (Training Set)
SMILES: O=C(O)CCC(C)C2CCC3C4CCC1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.602
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

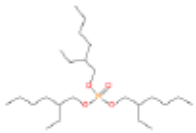
Compound #2

CAS: 103-23-1
Dataset id:52 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.597
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): SA41 Substituted n-alkylcarboxylic acids; SA42 Phthalate diesters and monoesters

Compound #3

CAS: 1643-20-5
Dataset id:879 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.597
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #4

CAS: 78-42-2
Dataset id:69 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.595
Experimental value : Carcinogen
Predicted value : Carcinogen

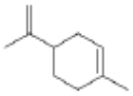
Alerts (not found also in the target): SA41 Substituted n-alkylcarboxylic acids

Compound #5

CAS: 75881-20-8
Dataset id:579 (Training Set)
SMILES: O=NN(C)CCCCCCCCCCCCCC
Similarity: 0.581
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): SA21 Alkyl and aryl N-nitroso groups

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 5989-27-5
Dataset id:267 (Training Set)
SMILES: C=C(C)C1CC=C(C)CC1
Similarity: 0.58
Experimental value : Carcinogen
Predicted value : NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.652
Explanation: The predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.599
Explanation: No similar compounds with known experimental value in the training set have been found..

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: Accuracy of prediction for similar molecules found in the training set is good..

Concordance for similar molecules
Concordance index = 0.504
Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value..

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.
The feature has a non optimal assessment, this aspect should be reviewed by an expert.
The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is Possible NON-Carcinogen, but the result may be not reliable.
A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC(CCCCCCCC)CC(C)CCCCCCCC
Experimental value: -
Predicted Carcinogenic activity: Possible NON-Carcinogen
No. alerts for carcinogenicity: 0
Structural Alerts: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

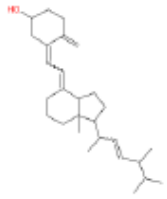
CAS: 63449-39-8
Dataset id:810 (Training Set)
SMILES: CCCC(CCCC(CCC(CCC(CCC(CCCC(CCC)Cl)Cl)Cl)Cl)Cl)Cl
Similarity: 0.634
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 18

Compound #2

CAS: 108171-27-3
Dataset id:675 (Training Set)
SMILES: CC(CCCC(CCCC(CCCC(CCCC(CCCC(CCCl)Cl)Cl)Cl)Cl)Cl)Cl
Similarity: 0.622
Experimental value : Carcinogen
Predicted value : Carcinogen

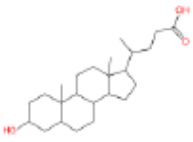
Alerts (not found also in the target): Carcinogenity alert no. 18



Compound #3

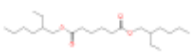
CAS: 50-14-6
Dataset id:806 (Training Set)
SMILES: OC3CC(=CC=C1CCCC2(C)(C1CCC2(C(C=CC(C)C(C)C)C)))C(=C)CC3
Similarity: 0.615
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 5; Carcinogenity alert no. 13; Carcinogenity alert no. 39



Compound #4

CAS: 434-13-9
Dataset id:93 (Training Set)
SMILES: O=C(O)CCC(C)C2CCC3C4CCC1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.602
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen



Compound #5

CAS: 103-23-1
Dataset id:43 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.597
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 29

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #6

CAS: 1643-20-5
Dataset id:777 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.597
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.623 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✖	Concordance for similar molecules Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✔	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✔ The feature has a good assessment, model is reliable regarding this aspect.
⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.
✖ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0 -

Prediction: Reliability:

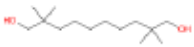
Prediction is Possible NON-Carcinogen, but the result shows some critical aspects, which require to be checked:
- Only moderately similar compounds with known experimental value in the training set have been found

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC(CCCCCCCC)CC(C)CCCCCCCC
Experimental value: -
Predicted Carcinogenic activity: Possible NON-Carcinogen
No. alerts for carcinogenicity: 0
Structural Alerts: -
Reliability: The predicted compound could be out of the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 7235-40-7
Dataset id:130 (Training Set)
SMILES:
C(=CC=C(C=CC=C(C=CC1=C(C)CCCC1(C)C)C)C)C=C(C=CC=C(C=CC2=C(C)CCCC2(C)C)C)C
Similarity: 0.634
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

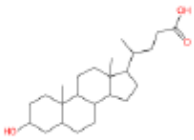


Compound #2

CAS: 35449-36-6
Dataset id:345 (Training Set)
SMILES: OCC(C)(C)CCCCCCC(C)(C)CO
Similarity: 0.611
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

Compound #3

CAS: 79-81-2
Dataset id:693 (Training Set)
SMILES: O=C(OCC=C(C=CC=C(C=CC1=C(C)CCCC1(C)C)C)C)CCCCCCCCCCCCCCCC
Similarity: 0.604
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen



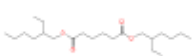
Compound #4

CAS: 434-13-9
Dataset id:413 (Training Set)
SMILES: O=C(O)CCC(C)C2CCC3C4CCC1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.602
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

Compound #5

CAS: 1643-20-5
Dataset id:273 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.597
Experimental value : NON-Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 64



Compound #6

CAS: 103-23-1
Dataset id:315 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.597
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

⚠	Global AD Index AD index = 0.785 Explanation: The predicted compound could be out of the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.616 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✓	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✓	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✓	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC(CCCCCCCC)CC(C)CCCCCCCC
Experimental value: -
Predicted Oral Carcinogenic class: Carcinogen
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 124-18-5
Dataset id:425 (Training Set)
SMILES: CCCCCCCCCC
Similarity: 0.756
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #2

CAS: 111-84-2
Dataset id:610 (Training Set)
SMILES: CCCCCCCCC
Similarity: 0.735
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #3

CAS: 30501-43-0
Dataset id:692 (Training Set)
SMILES: CC1(C)(CCCCC1(C)(C))
Similarity: 0.69
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #4

CAS: 108-87-2
Dataset id:587 (Training Set)
SMILES: CC1CCCCC1
Similarity: 0.637
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #5

CAS: 110-54-3
Dataset id:540 (Training Set)
SMILES: CCCCCC
Similarity: 0.631
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #6

CAS: 96-37-7
Dataset id:588 (Training Set)
SMILES: CC1CCCC1
Similarity: 0.603
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.745 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✖	Concordance for similar molecules Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✔	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✔	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC(CCCCCCCC)CC(C)CCCCCCCC
Experimental value: -
Predicted Inhalation Carcinogenic class: Carcinogen
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 124-18-5
Dataset id:389 (Training Set)
SMILES: CCCCCCCCCC
Similarity: 0.756
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #2

CAS: 111-84-2
Dataset id:593 (Training Set)
SMILES: CCCCCCCCC
Similarity: 0.735
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #3

CAS: 30501-43-0
Dataset id:687 (Training Set)
SMILES: CC1(C)(CCCCC1(C)(C))
Similarity: 0.69
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #4

CAS: 108-87-2
Dataset id:567 (Training Set)
SMILES: CC1CCCCC1
Similarity: 0.637
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #5

CAS: 110-54-3
Dataset id:516 (Training Set)
SMILES: CCCCCC
Similarity: 0.631
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #6

CAS: 96-37-7
Dataset id:568 (Training Set)
SMILES: CC1CCCC1
Similarity: 0.603
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.745 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✖	Concordance for similar molecules Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✔	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✔	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

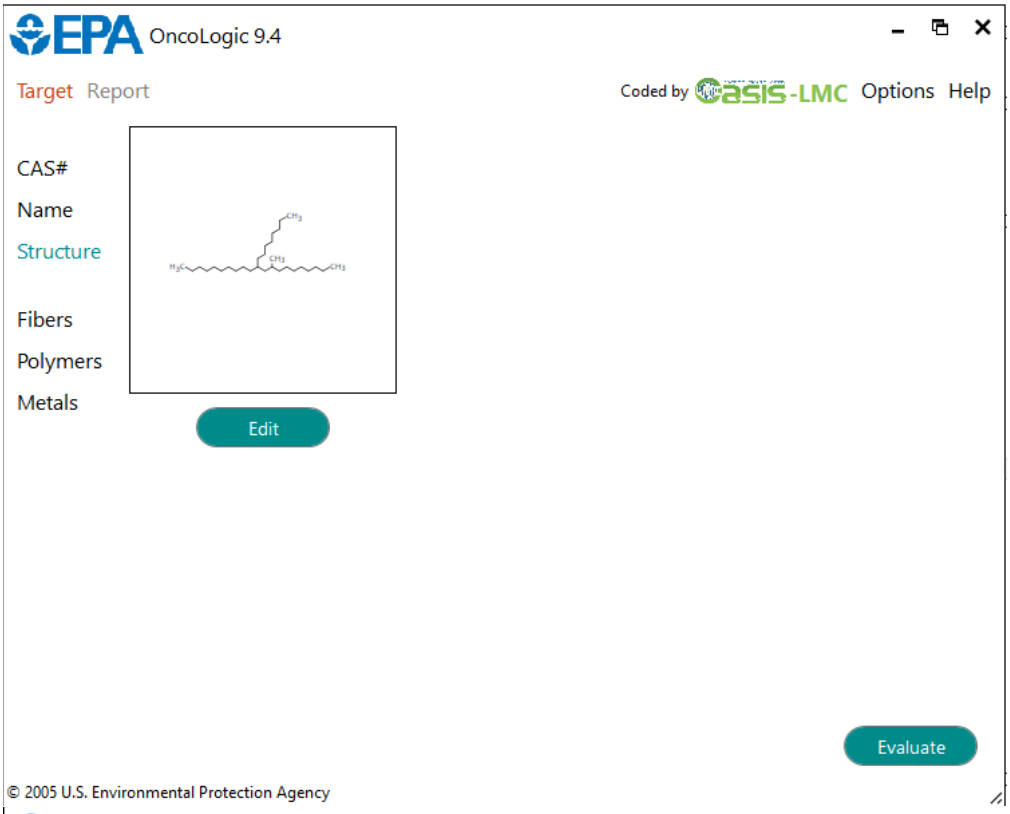
Symbols explanation:

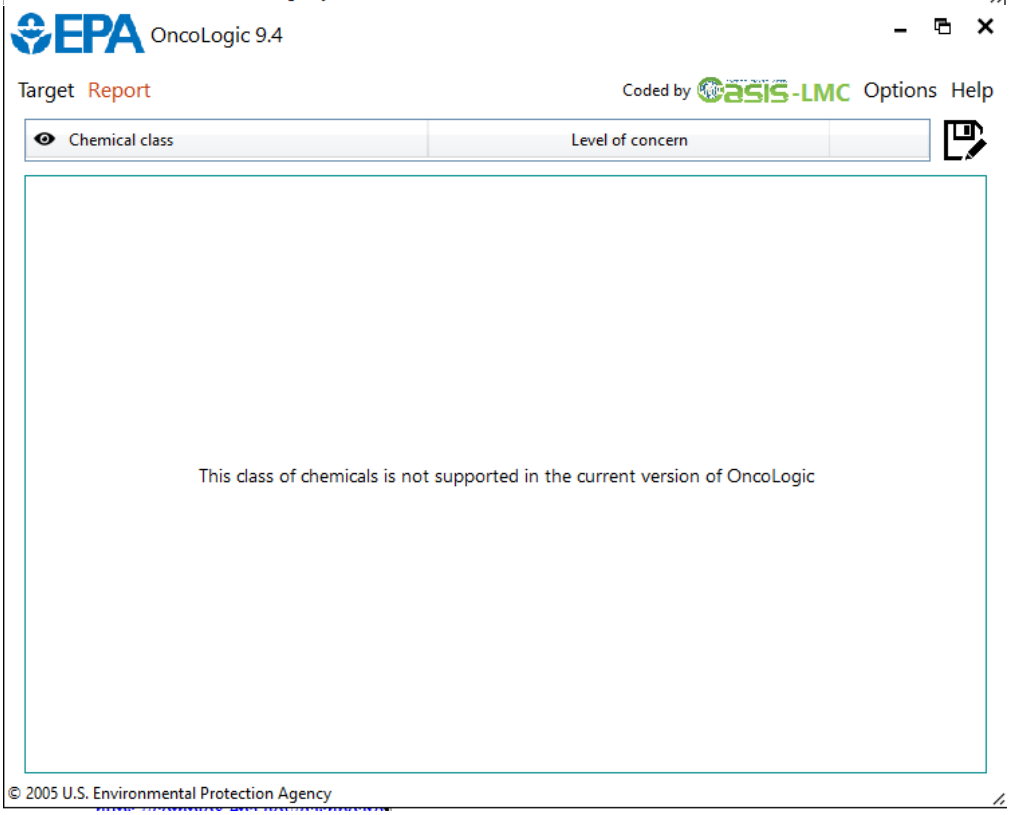
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

APPENDIX E: OncoLogic Results for the Hydrogenated 1-Decene Trimer



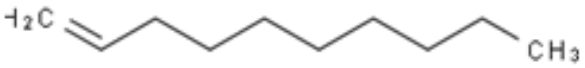


APPENDIX F: Danish QSAR Carcinogenicity Prediction Results for Hydrogenated Polydecene (CAS #68037-01-4)

Danish (Q)SAR Database, https://qsar.food.dtu.dk Date: 21-03-2025

(Q)SAR predicted profile

Structure (as used for QSAR prediction):



SMILES (used for QSAR prediction): C(=C)CCCCCCCC

ID

Registry Number	68037-01-4	PubChem CID	
REACH EC Number (pre-registration, by 2013)	500-183-1	REACH EC Number (registration, 2019 or 2022)	500-183-1
REACH registration (2022)	Yes	REACH registration cumulated minimum annual tonnage (2022)	10000
EU CLP Harmonized Classification*		DK-EPA / DTU QSAR-based CLP Advisory Classification	Acute Tox. 4; Aquatic Acute 1
EU Biocide active substances		EU Pesticide active substances	
EU EFSA Botanical substances		US TSCA (Oct. 2021)	Yes
Tox21 (2019)		ToxCast (Oct. 2021)	
Molecular Formula	C10 H20	Molecular weight (g/mole)	140.27
Chemical Name	Dec-1-ene, homopolymer, hydrogenated Dec-1-ene, oligomers, hydrogenated		

(Annex VI to CLP up to and including the 9th ATP, and including Nordic Council of Minister SPIN list for group entries)

Carcinogenicity

	68037-01-4E Ultra	Leadscope
FDA RCA Cancer Male Rat	NEG_IN	NEG_IN
FDA RCA Cancer Female Rat	NEG_IN	NEG_IN
FDA RCA Cancer Rat	NEG_IN	NEG_IN
FDA RCA Cancer Male Mouse	NEG_IN	INC_OUT
FDA RCA Cancer Female Mouse	POS_IN	INC_OUT
FDA RCA Cancer Mouse	NEG_IN	NEG_IN
FDA RCA Cancer Rodent	NEG_IN	NEG_IN

Commercial models from CASE Ultra and Leadscope

FDA RCA: Data from US Food and Drug Administration as part of Research Cooperation Agreement

Carcinogenicity (genotox and nongenotox) alerts by ISS, alerts in:	
- parent only	No alert found
Oncologic Primary Classification, alerts in:	
- parent only	Not classified

OECD QSAR Toolbox v.4.2 profilers

Profiler predictions are supporting information to be used together with the relevant QSAR predictions

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Liver Specific Cancer in Rat or Mouse		NEG_IN	NEG_IN	NEG_IN	NEG_IN

DTU-developed models

APPENDIX G: EPI Suite™ Modeling Results for Hydrogenated 1-Decene Hexamer

CAS Number:
SMILES :
CCCCCCCCCCC(CCCCCCCC)CC(CCCCCCCC)CC(CCCCCCCC)CC(CCCCCCCC)CC(C)CCCCCCC
C
CHEM :
MOL FOR: C60 H122
MOL WT : 843.64
---------- EPI SUMMARY (v4.11) ----------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Water Solubility (mg/L): ------
Physical Property Inputs:
Vapor Pressure (mm Hg) : ------
Melting Point (deg C) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.69 estimate) = 29.44

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 763.60 (Adapted Stein & Brown method)
Melting Pt (deg C): 335.73 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 6.31E-018 (Modified Grain method)
VP (Pa, 25 deg C) : 8.41E-016 (Modified Grain method)
Subcooled liquid VP: 2.12E-014 mm Hg (25 deg C, Mod-Grain method)
: 2.83E-012 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 7.976e-026
log Kow used: 29.44 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 8.4364e-007 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 7.54E+006 atm-m3/mole (7.64E+011 Pa-m3/mole)
Group Method: 5.35E+008 atm-m3/mole (5.42E+013 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.392E+010 atm-m3/mole (1.410E+015 Pa-m3/mole)

VP: 1E-015 mm Hg (source: MPBPVP)
WS: 7.98E-026 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 29.44 (KowWin est)
Log Kaw used: 8.489 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 20.951
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.9965
Biowin2 (Non-Linear Model) : 0.8900
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.1249 (weeks)
Biowin4 (Primary Survey Model) : 4.2450 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.4045
Biowin6 (MITI Non-Linear Model): 0.1795
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): -1.2090
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
LOG BioHC Half-Life (days) : 4.4538
BioHC Half-Life (days) : 28429.5195

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 2.83E-012 Pa (2.12E-014 mm Hg)
Log Koa (Koawin est): 20.951
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 1.06E+006
Octanol/air (Koa) model: 2.19E+008
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 1
Mackay model : 1
Octanol/air (Koa) model: 1

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 84.7873 E-12 cm3/molecule-sec
Half-Life = 0.126 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 1.514 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
1 (Junge-Pankow, Mackay avg)
1 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 1E+010 L/kg (MCI method)
Log Koc: 15.997 (MCI method)
Koc : 3.553E+025 L/kg (Kow method)
Log Koc: 25.551 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 7.4730 days (HL = 2.972e+007 days)
Log BCF Arnot-Gobas method (upper trophic) = -0.049 (BCF = 0.893)
Log BAF Arnot-Gobas method (upper trophic) = -0.049 (BAF = 0.893)
log Kow used: 29.44 (estimated)

Volatilization from Water:
Henry LC: 7.54E+006 atm-m3/mole (estimated by Bond SAR Method)
Half-Life from Model River: 2.964 hours
Half-Life from Model Lake : 275.9 hours (11.5 days)

Removal In Wastewater Treatment:
Total removal: 94.04 percent
Total biodegradation: 0.78 percent
Total sludge adsorption: 93.26 percent
Total to Air: 0.00 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model: (MCI Method)
** Note: When the Log Kow is > 7, the model may be underestimating the mass of material in sediment and overestimating the mass of material in the water column (biota). Consider using the results of the default EQC model. **

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.22	3.03	1000
Water	94.6	360	1000
Soil	3.21	720	1000
Sediment	2.03e-015	3.24e+003	0

Persistence Time: 123 hr

Level III Fugacity Model: (MCI Method with Water percents)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.22	3.03	1000
Water	94.6	360	1000
water	(6.87e-021)		
biota	(94.6)		

suspended sediment (1.03e-016)
Soil 3.21 720 1000
Sediment 2.03e-015 3.24e+003 0
Persistence Time: 123 hr

Level III Fugacity Model: (EQC Default)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0966	3.03	1000
Water	3.65	360	1000
water	(2e-023)		
biota	(0.275)		
suspended sediment	(3.38)		
Soil	29.7	720	1000
Sediment	66.6	3.24e+003	0

Persistence Time: 1.28e+003 hr

APPENDIX H: EPI Suite™ Modeling Results for Hydrogenated 1-Decene Trimer

CAS Number:
SMILES : CCCCCCCCCCC(CCCCCCCC)CC(C)CCCCCCCC
CHEM :
MOL FOR: C30 H62
MOL WT : 422.83
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.69 estimate) = 14.93

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 436.47 (Adapted Stein & Brown method)
Melting Pt (deg C): 132.95 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 2.3E-007 (Modified Grain method)
VP (Pa, 25 deg C) : 3.06E-005 (Modified Grain method)
Subcooled liquid VP: 2.78E-006 mm Hg (25 deg C, Mod-Grain method)
: 0.000371 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 1.145e-010
log Kow used: 14.93 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 4.2283e-007 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 1.53E+003 atm-m3/mole (1.55E+008 Pa-m3/mole)
Group Method: 9.74E+003 atm-m3/mole (9.87E+008 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.118E+003 atm-m3/mole (1.132E+008 Pa-m3/mole)
VP: 2.3E-007 mm Hg (source: MPBPVP)
WS: 1.15E-010 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 14.93 (KowWin est)
Log Kaw used: 4.796 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 10.134
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.8715
Biowin2 (Non-Linear Model) : 0.9266
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.1598 (weeks)
Biowin4 (Primary Survey Model) : 4.0449 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.5303
Biowin6 (MITI Non-Linear Model): 0.5794
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): -0.1433
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
LOG BioHC Half-Life (days) : 2.2778
BioHC Half-Life (days) : 189.5975

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 0.000371 Pa (2.78E-006 mm Hg)
Log Koa (Koawin est): 10.134
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.00809
Octanol/air (Koa) model: 0.00334
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.226
Mackay model : 0.393
Octanol/air (Koa) model: 0.211

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 40.3347 E-12 cm3/molecule-sec
Half-Life = 0.265 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 3.182 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
0.31 (Junge-Pankow, Mackay avg)
0.211 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 1.922E+008 L/kg (MCI method)
Log Koc: 8.284 (MCI method)

Koc : 9.065E+012 L/kg (Kow method)
Log Koc: 12.957 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 3.2473 days (HL = 1767 days)
Log BCF Arnot-Gobas method (upper trophic) = -0.049 (BCF = 0.8938)
Log BAF Arnot-Gobas method (upper trophic) = 0.681 (BAF = 4.797)
log Kow used: 14.93 (estimated)

Volatilization from Water:
Henry LC: 1.53E+003 atm-m3/mole (estimated by Bond SAR Method)
Half-Life from Model River: 2.098 hours
Half-Life from Model Lake : 195.3 hours (8.138 days)

Removal In Wastewater Treatment:
Total removal: 94.04 percent
Total biodegradation: 0.78 percent
Total sludge adsorption: 93.26 percent
Total to Air: 0.00 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model: (MCI Method)
** Note: When the Log Kow is > 7, the model may be underestimating the mass of material in sediment and overestimating the mass of material in the water column (biota). Consider using the results of the default EQC model. **

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.56	6.36	1000
Water	41.6	360	1000
Soil	56.8	720	1000
Sediment	0.00556	3.24e+003	0

Persistence Time: 276 hr

Level III Fugacity Model: (MCI Method with Water percents)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.56	6.36	1000
Water	41.6	360	1000
water	(9.79e-007)		
biota	(41.6)		
suspended sediment	(0.000282)		
Soil	56.8	720	1000
Sediment	0.00556	3.24e+003	0

Persistence Time: 276 hr

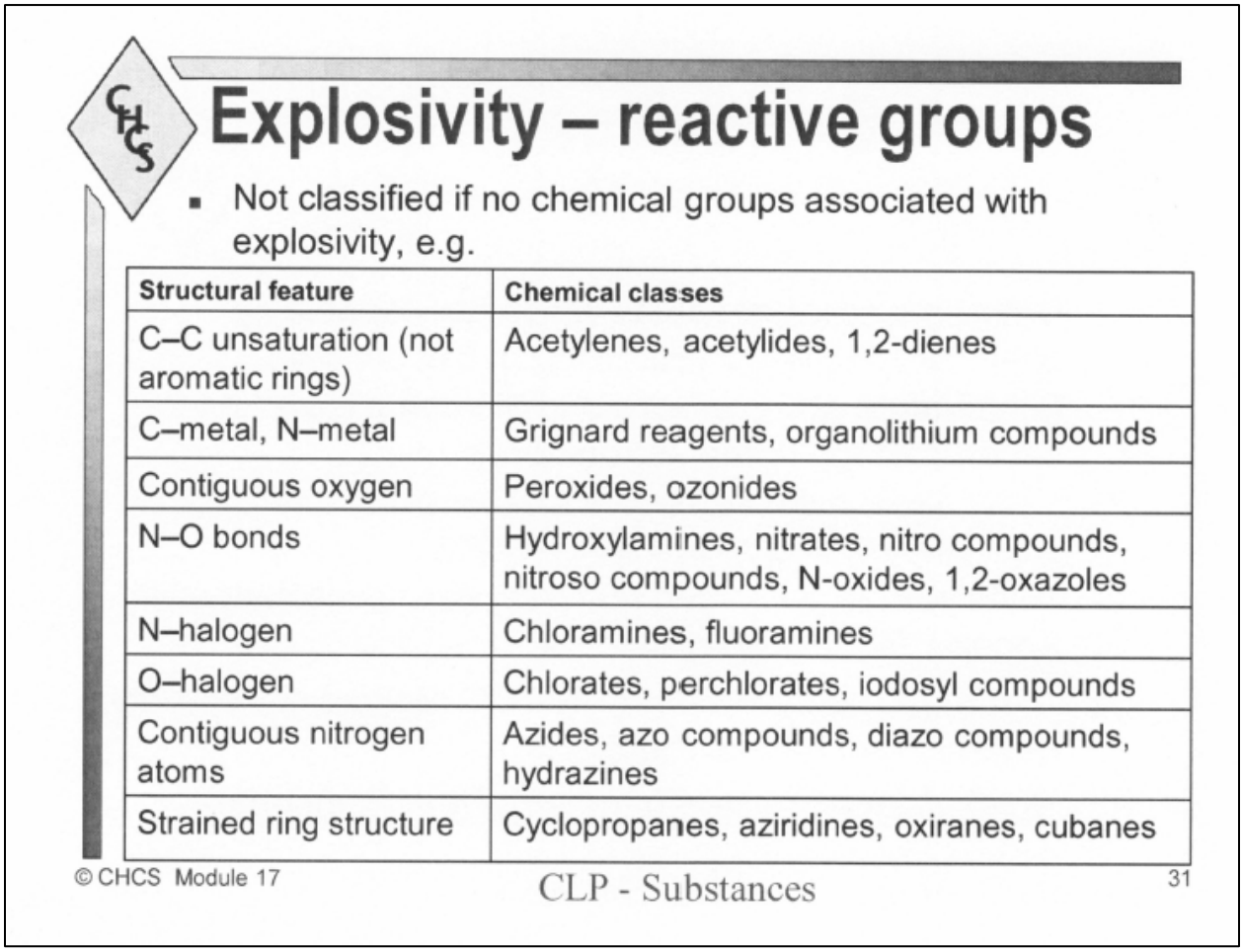
Level III Fugacity Model: (EQC Default)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.209	6.36	1000
Water	3.69	360	1000
water	(6.52e-009)		
biota	(0.278)		
suspended sediment	(3.41)		
Soil	28.9	720	1000
Sediment	67.2	3.24e+003	0

Persistence Time: 1.26e+003 hr

APPENDIX I: Known Structural Alerts for Reactivity

Explosivity – Abbreviated List



Explosivity – reactive groups

- Not classified if no chemical groups associated with explosivity, e.g.

Structural feature	Chemical classes
C–C unsaturation (not aromatic rings)	Acetylenes, acetylides, 1,2-dienes
C–metal, N–metal	Grignard reagents, organolithium compounds
Contiguous oxygen	Peroxides, ozonides
N–O bonds	Hydroxylamines, nitrates, nitro compounds, nitroso compounds, N-oxides, 1,2-oxazoles
N–halogen	Chloramines, fluoramines
O–halogen	Chlorates, perchlorates, iodosyl compounds
Contiguous nitrogen atoms	Azides, azo compounds, diazo compounds, hydrazines
Strained ring structure	Cyclopropanes, aziridines, oxiranes, cubanes

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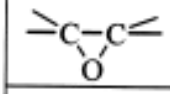
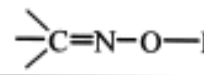
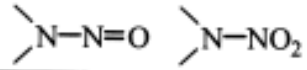
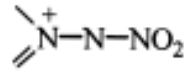
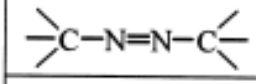
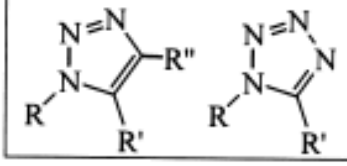
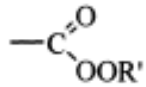
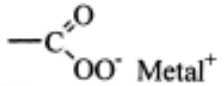
Explosivity – Full List

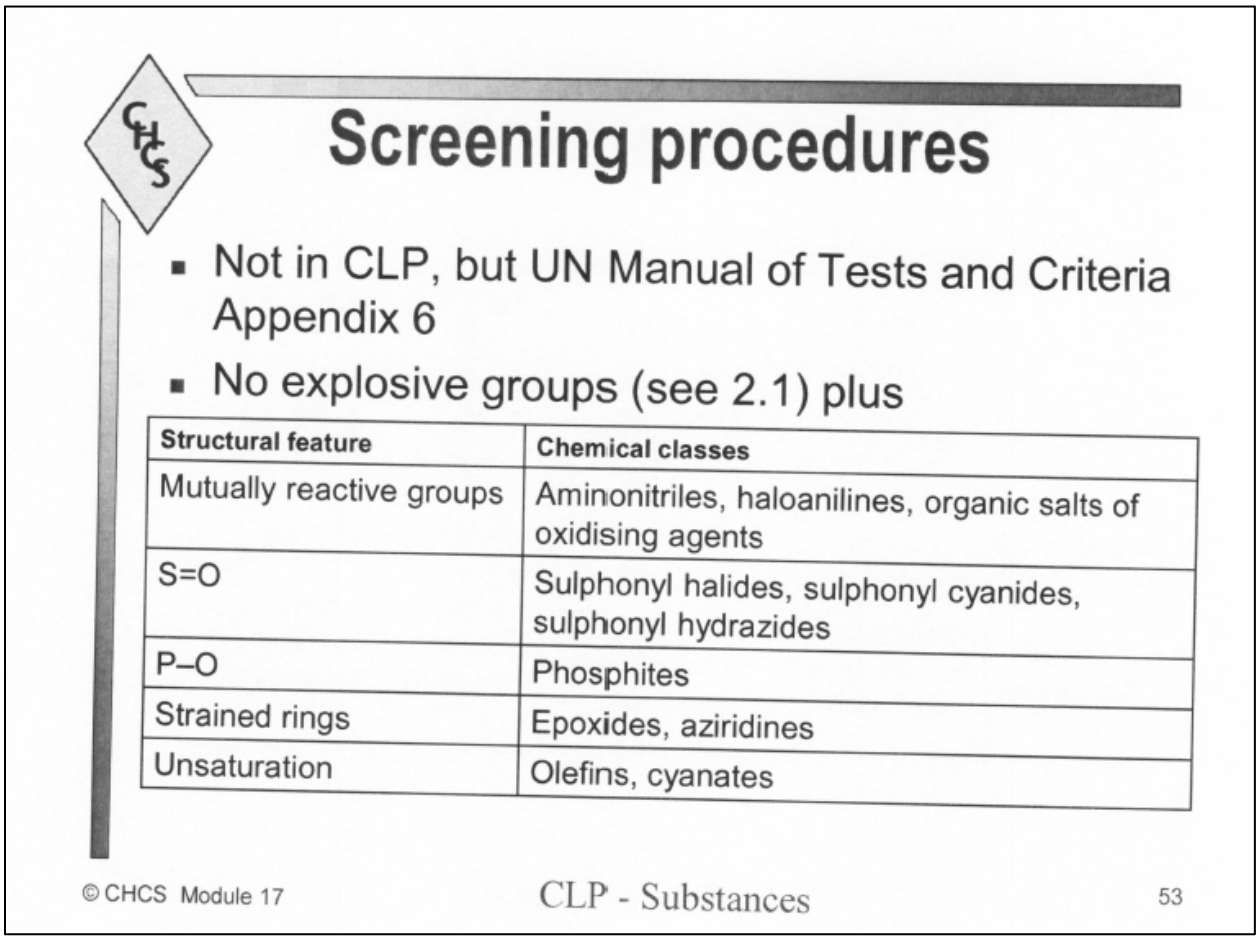
Table R.7.1-28 Chemical groups associated with explosive properties

Chemical group	Chemical Class
-C≡C- -C≡C-Metal -C≡C-Halogen	Acetylenic Compounds Metal Acetylides Haloacetylene Derivatives
	Diazo Compounds
-N=O -NO_2	Nitroso and Nitro Compounds,
R-O-N=O R-O-NO_2	Acyl or Alkyl Nitrites and Nitrates
	1,2-Epoxides
	Metal Fulminates or *aci*-Nitro Salts
	N-Metal Derivatives (especially heavy metals)
	N-Nitroso and N-Nitro Compounds
	N-Azolium Nitroimidates
	Azo Compounds
Ar-N=N-O-Ar	Arene Diazoates
$(ArN=N)_2O$, $(ArN=N)_2S$	Bis-Arenediazo Oxides and Sulfides
RN=N-NR'R''	Triazines
	High-nitrogen Compounds: e.g. Triazoles, Tetrazoles

Chemical group	Chemical Class
[1] ROOR', [2] 	Peroxy Compounds: [1] Alkyl hydroperoxides (R'=H), Peroxides (R'=organic); [2] Peroxo acids (R'=H), Peroxyesters (R'=organic)
[1] ROOMetal, [2] 	Metal peroxides, Peroxoacids salts
$-N_3$	Azides e.g. PbN_6, CH_3N_3
$^-O-C-N_2^+$	Arenediazonium oxides i.e. inner diazonium salts in which the counter ion is an oxide
Ar-N=N-S- Ar-N=N-S-Ar	Diazonium sulfides and derivatives, Arenediazo Aryl Sulfides
XO_n	Halogen Oxide: e.g. percholrates, bromates, etc
NX_3 e.g. $NC1_3$, $RNC1_2$	N-Halogen Compounds

Adapted from Bretherick (Bretherick's Handbook of Reactive Chemical Hazards 6th Ed., 1999, Butterworths, London)

Self-Reactive Substances



APPENDIX J: Change in Benchmark Score

Table 5 provides a summary of changes to the GreenScreen® Benchmark™ for hydrogenated polydecene. The Benchmark score of hydrogenated polydecene has changed over time. The original GreenScreen® assessment was performed in March 2025 under version 1.4 criteria and ToxServices assigned a Benchmark 3 (BM-3) score. This BM score is updated to 2 in a subsequent revision due to re-evaluation of its aspiration hazard.

Table 5: Change in GreenScreen® Benchmark™ for Hydrogenated polydecene

Date	GreenScreen® Benchmark™	GreenScreen® Version	Comment
March 21, 2025	BM-3	v. 1.4	Original GreenScreen® assessment.
July 8, 2025	BM-2	v. 1.4	BM score changed from 3 to 2 due to re-evaluation of aspiration hazard in the single exposure systemic toxicity endpoint, leading to an updated hazard score of **High** (high confidence) instead of **Low** (high confidence).

Licensed GreenScreen® Profilers

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