ECOSOLV (CAS# 68551-19-9)
Certified GreenScreen® Assessment

Prepared for
Alex Stone, Sc.D.
Washington Department of Ecology
Hazardous Waste & Toxics Reduction-HQ
P.O. Box 47600
Olympia WA 98504-7600

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GRADIENT

www.gradientcorp.com
20 University Road
Cambridge, MA 02138
617-395-5000

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GreenScreen® Assessment for ECOSOLV (CAS# 68551-19-9)

Method Version: GreenScreen Version 1.3[1]

Assessment Type:[2] **Certified**

Chemical Name: ECOSOLV

GreenScreen Assessment Prepared By:	GreenScreen Assessment Quality Control Performed By:
Name: Jiaru Zhang	Name: Ari Lewis, Tom Lewandowski
Title: Senior Health Scientist	Title: Principals/Toxicologists
Organization: Gradient	Organization: Gradient
Date: 9/30/2016	Date: 9/30/2016
Name: Daniel Skall	Name: Tim Verslycke
Title: Environmental Toxicologist	Title: Principal
Organization: Gradient	Organization: Gradient
Date: 9/30/2016	Date: 9/30/2016
Name: Chase Butler	Name: Kim Reid
Title: Environmental Chemist	Title: Principal Scientist
Organization: Gradient	Organization: Gradient
Date: 9/30/2016	Date: 9/30/2016
Assessor Type (Licensed GreenScreen Profiler, Authorized GreenScreen Practitioner or Unaccredited):	Licensed GreenScreen Profiler

[1] Use GreenScreen Assessment Procedure (Guidance) v1.3 (March 2016).
[2] GreenScreen reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen Practitioner), "CERTIFIED" (by Licensed GreenScreen Profiler or equivalent) or "CERTIFIED WITH VERIFICATION" (Certified or Authorized assessment that has passed GreenScreen Verification Program).

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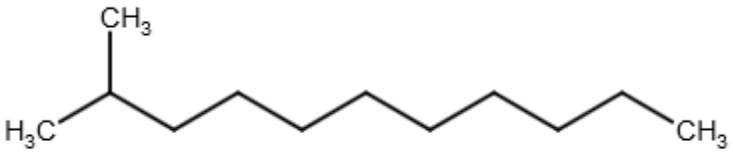
Confirm Application of the Disclosure and Assessment Rules and Best Practice:[3] N/A

Chemical Name (CAS#): ECOSOLV (CAS# 68551-19-9)

Also Called:

C12-14 Isoparaffin; Alkanes, C12-14-iso-

Chemical Structure:



(representative C12 structure; some component of ECOSOLV may be more highly branched)

Suitable Analogs or Moieties Used in This Assessment (CAS #):

Solvent naphtha (petroleum), medium aliphatic (Chemistry Abstracts Service [CAS]# 64742-88-7);[4] C9-12 Isoparaffin (CAS# 90622-57-4);[5] Isododecane (CAS# 141-70-8); C10-11 Isoparaffin (CAS# 246538-75-0); C11-13 Isoparaffin (CAS# 246538-78-3); C10-13 Isoparaffin (CAS# 68551-17-7); Pristane (CAS# 1921-70-6); and 2,2,4,6,6-Pentamethylheptane (CAS# 13475-82-6), Hydrocarbons, C10-C12, containing isoalkanes with < 2% aromatics (no CAS#), Hydrocarbons, C11-12, isoalkanes, with < 2% aromatics (no CAS#).

Several surrogates were identified to assist in filling data gaps for multiple endpoints, as indicated in Table 1. These compounds are considered appropriate and relevant surrogates because, like ECOSOLV, they contain branched, saturated hydrocarbons (alkanes), and their component substances contain only carbon-carbon (C-C) and carbon-hydrogen (C-H) bonds.[6] These surrogate substances are composed of alkanes with a similar number of carbons as the alkanes in ECOSOLV, and thus are expected to exhibit similar physicochemical properties to ECOSOLV *in vivo* and in the environment.

Chemical Structure(s):

Most of the surrogates used in this assessment are, like ECOSOLV, mixtures of unknown and variable composition. Representative structures are shown below; the actual substances may contain compounds of different sizes and connectivities.

[3] See GreenScreen Guidance v1.3.
[4] In the toxicity studies of this substance, it is described as "composed primarily of C10-C13 aliphatic constituent [sic] with < 1% aromatics" and "C10-C13 n-alkanes, isoalkanes, cyclic" (OECD, 2012).
[5] In some toxicity studies of this substance, it is described as "C10-C12 isoalkanes" (OECD, 2012).
[6] Some hydrocarbon mixtures contain aromatic components (*e.g.*, benzene, ethylbenzene, *etc.*); based on the information we have been able to obtain, ECOSOLV is not reported to contain aromatic compounds.

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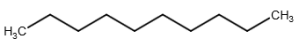
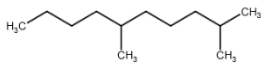
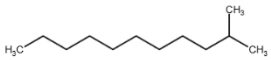
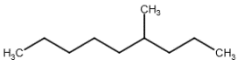
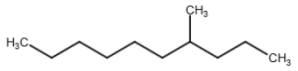
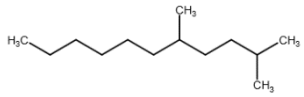
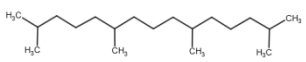
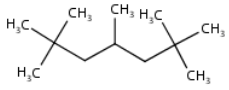
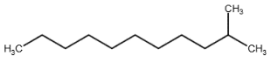
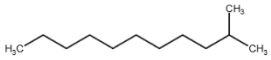
Table 1 Chemical Structures of Surrogates Used in the GreenScreen Assessment of ECOSOLV (CAS# 68551-19-9)

Surrogate Name (CAS#)	Representative Structure	Endpoint Assessed
Solvent Naphtha (petroleum), Medium Aliphatic (CAS# 64742-88-7)[4]		Carcinogenicity, Mutagenicity/Genotoxicity, Acute and Chronic Aquatic Toxicity, Persistence, Bioaccumulation, Partition Coefficient (log K_{ow})
C9-12 Isoparaffin (CAS# 90622-57-4)[5]		Mutagenicity/Genotoxicity, Acute and Chronic Aquatic Toxicity, Persistence, Bioaccumulation, Partition Coefficient (log K_{ow})
Isododecane (CAS# 141-70-8)		Reproductive Toxicity, Systemic Toxicity/Organ Effects (Repeated Dose)
C10-11 Isoparaffin (CAS# 246538-75-0)		Developmental Toxicity, Acute Oral Toxicity, Acute Dermal Toxicity, Acute Inhalation Toxicity, Skin Sensitization, Skin Irritation, Eye Irritation
C11-13 Isoparaffin (CAS# 246538-78-3)		Acute Oral Toxicity, Acute Dermal Toxicity, Acute Inhalation Toxicity, Skin Sensitization, Skin Irritation, Eye Irritation
C10-13 Isoparaffin (CAS# 68551-17-7)		Acute Oral Toxicity, Acute Dermal Toxicity, Acute Inhalation Toxicity, Skin Sensitization, Skin Irritation, Eye Irritation, Acute and Chronic Aquatic Toxicity
Pristane (CAS# 1921-70-6)		Transformation products
2,2,4,6,6-Pentamethylheptane (CAS# 13475-82-6)		Acute and Chronic Aquatic Toxicity, Bioaccumulation, Partition Coefficient (log K_{ow})
Hydrocarbons, C10-C12, Containing Isoalkanes with < 2% Aromatics (no CAS#)		Neurotoxicity (single exposure), Acute and Chronic Aquatic Toxicity, Persistence
Hydrocarbons, C11-12, Isoalkanes, with < 2% Aromatics (no CAS#)		Neurotoxicity (single exposure)

Note:
CAS = Chemistry Abstracts Service.

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Notes Related to Production Specific Attributes:[7] Not Applicable

Identify Applications/Functional Uses:

1. Dry cleaning fluid (Chevron, 2014)
2. Solvent for automotive products, paintings and coatings, degreasers, floor wax (OECD, 2012)
3. Diluent in asphalt applications (OECD, 2012)
4. Pesticide carrier base (OECD, 2012)

GreenScreen Benchmark Score and Hazard Summary Table:[8,9,10,11]

ECOSOLV is assigned a **Benchmark Score of 1** based on moderate carcinogenicity, very high chronic aquatic toxicity, and very high bioaccumulation (Table 2). Although data gaps were evident for endocrine activity, systemic toxicity-single exposure, neurotoxicity-repeated exposure, and respiratory sensitization, all data requirements were met for Benchmark 1 classification.

If we consider the worst case benchmarking scenario based on the reported data gaps, endocrine activity would be designated high (H), systemic toxicity-single exposure would be designated very high (vH), neurotoxicity-repeated exposure would be designated high (H), and respiratory sensitization would be designated a high hazard (H). Even under this worst case scenario, ECOSOLV would still receive a Benchmark 1 classification.

Table 2 GreenScreen (v1.3) Hazard Profile Summary Table – ECOSOLV (CAS# 68551-19-9)

Group I Human					Group II and II* Human									Ecotox		Fate		Phys	
C	M	R	D	E	AT	ST		N		SnS *	SnR *	IrS	IrE	AA	CA	P	B	Rx	F
						sgl	rpt*	sgl	rpt*										
M	**L**	*L*	*L*	*dg*	**L**	*dg*	*L*	*M*	*dg*	*L*	*dg*	*H*	*M*	*L*	*vH*	*H*	**vH**	*L*	**M**

Notes:
CAS = Chemistry Abstracts Service.
Hazard levels (Very High [vH], High [H], Moderate [M], Low [L], Very Low [vL]) in *italics* reflect estimated values, authoritative B lists, screening lists, weak analogues, and lower confidence.
Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues.
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.

[7] Note any composition or hazard attributes of the chemical product relevant to how it is manufactured. For example, certain synthetic pathways or processes result in typical contaminants, by-products or transformation products. Explain any differences between the manufactured chemical product and the GreenScreen assessment of the generic chemical by CAS#.
[8] See Appendix A for a glossary of hazard endpoint acronyms.
[9] See Appendix B for the PHAROS results for ECOSOLV and its transformation products.
[10] For inorganic chemicals only, see GreenScreen Guidance v1.3 Section 13. (Exceptions for Persistence).
[11] 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 v1.3 Section 8.2.1.

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Environmental Transformation Products and Ratings:[12]

Identify feasible and relevant environmental transformation products (*i.e.*, dissociation products, transformation products, valence states) and/or moieties of concern:[13]

Table 3 Environmental Transformation Products and Ratings

Functional Use	Life Cycle Stage	Transformation Pathway	Environmental Transformation Products	CAS#	Feasible and Relevant?	GreenScreen List Translator Score
N/A	End	Microbial Oxidation	Undecanoic Acid, 10-Methyl-	2724-56-3	Yes	Not Listed
N/A	End	Microbial Oxidation	2-Methylglutaric Acid	18069-17-5	Yes	Not Listed

Notes:
CAS = Chemistry Abstracts Service; N/A = Not Applicable.

As saturated hydrocarbons, the components of ECOSOLV are not readily transformed by chemical reactions under ambient conditions (Labinger and Bercaw, 2002). Saturated hydrocarbons do not contain hydrolysable functional groups; thus, hydrolysis is not a significant fate process for the components of ECOSOLV (ECHA, 2015). Similarly, saturated hydrocarbons do not absorb radiation at wavelengths > 290 nm and thus are not susceptible to transformation *via* photolysis under ambient conditions (ECHA, 2015).

The components of ECOSOLV may, however, be susceptible to biodegradation by microorganisms. The linear portions of the hydrocarbons in ECOSOLV may be the most readily degraded, with biodegradation occurring at the chain end to form an alkyl carboxylic acid. Further biodegradation of alkyl carboxylic acids would lead to shorter-chain acids (by two methylene units) and carbon dioxide. Components of ECOSOLV containing high degrees of methyl branching (particularly terminal methyl branching) may be more resistant to microbial attack (Atlas, 1981). Still, highly branched hydrocarbons such as pristane (CAS# 1921-70-6) have been found to undergo microbial degradation to form dicarboxylic acids (Atlas, 1981; McKenna and Kallio, 1971).

Table 3 lists two possible transformation products identified for ECOSOLV. The unknown and variable nature of ECOSOLV's components, combined with the complicated processes of microbial oxidation, make it difficult to predict the precise transformation products of ECOSOLV in the environment. In Table 3, undecanoic acid, 10-methyl- represents an initial oxidation of a representative component of ECOSOLV, in which the oxidation has occurred at a linear chain-end. The second transformation product in Table 3, 2-methylglutaric acid, is a dicarboxylic acid that was identified in the microbial degradation of pristane, a branched alkane that may have a structure similar to those of components of ECOSOLV.[14]

Summary

No specific transformation products of ECOSOLV were identified in the scientific literature reviewed, and the lack of reactive functional groups in the components of ECOSOLV likely render it generally inert

[12] See GreenScreen Guidance v1.3 Section 12.
[13] A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.
[14] However, pristane ($C_{19}H_{40}$) is larger than the hydrocarbons comprising ECOSOLV.

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under ambient environmental conditions. Oxidation by microorganisms may contribute to the degradation of ECOSOLV in the environment, and a couple potential products of such oxidations have been identified. These products were not listed in the Pharos List Translator. Full GreenScreen assessments of these compounds would be needed to better understand the hazards associated with products of ECOSOLV degradation and their impacts on ECOSOLV's Benchmark 1 score.

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Introduction

ECOSOLV is an industrial chemical that is used as a solvent in dry cleaning, automotive products, paints and coatings, degreasers, floor wax, and as a diluent for asphalt and a carrier for pesticides (Chevron, 2014; OECD, 2012). Table 4 summarizes the physical and chemical properties obtained for ECOSOLV.

Table 4 Physical and Chemical Properties of ECOSOLV (CAS# 68551-19-9)

Property	Value	Reference
Molecular Formula	C_nH_{2n+2}, where n = 12-14	
SMILES Notation	Not Applicable[a]	
Molecular Weight	170.34 – 198.40	
Physical State	Liquid	ECHA, 2015 Chevron, 2014
Appearance	Colorless	ECHA, 2015 Chevron, 2014
Melting Point	< -114°C	ECHA, 2015
Vapor Pressure	0.30 mm Hg at 20°C[b] 0.15 mm Hg at 38°C	ECHA, 2015 Chevron, 2014
Water Solubility	Negligible	Chevron, 2014
Dissociation Constant	Not Applicable[c]	
Density/Specific Gravity	0.76 g/cm^3 at 15°C 0.76 g/cm^3 at 15.6°C	ECHA, 2015 Chevron, 2014
Partition Coefficient, Log K_{ow}	ca. 3-7[d]	EC, ECB, 2000a-c

Notes:
ca. = Circa; Hg = Mercury; SMILES = Simplified Molecular-input Line-entry System.
Gradient assessed ECOSOLV against GreenScreen Version 1.3 (Clean Production Action, 2016).
(a) ECOSOLV (CAS# 68551-19-9) is an Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB) substance.
(b) Converted to mm Hg from the reported value, 0.04 kPa. This value was calculated *via* extrapolation from boiling range and density values.
(c) Not expected to dissociate based on lack of dissociative functional groups.
(d) See Table 16.

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Hazard Classification Summary Section

Hazard classifications for the GreenScreen endpoints evaluated are provided below.

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): *M*

ECOSOLV is assigned a score of *Moderate (M)* for carcinogenicity *via* the inhalation route based on results from two carcinogenicity studies conducted in two different species using a suitable surrogate. No oral or dermal carcinogenicity studies were located for ECOSOLV. The confidence level associated with this score is low because no study was identified that was conducted specifically with ECOSOLV.

Authoritative and Screening Lists

ECOSOLV

- *Authoritative*: Not listed
- *Screening*: Not listed

Surrogate: Solvent naphtha, (petroleum), medium aliphatic, composed of primarily C10-13 aliphatic with < 1% aromatic (CAS# 64742-88-7)

Direct Hazards:

- *Authoritative*: Not listed
- *Screening*: Not listed

Potential Residual Hazards (due to impurity):

- *Authoritative*:
  - Group 2b-Possibly carcinogenic to humans (International Agency for the Research of Cancer [IARC])
  - Group 4-Non-genotoxic carcinogen with low risk under MAK Commision of Germany Maximum Concentrations at the Workplace (MAK)/Biological Tolerance Values (BAT) levels
  - Carcinogen from ethylbenzene impurity (California Environmental Protection Agency [CalEPA] Proposition 65)
  - Inadequate information to assess carcinogenic potential (United States Environmental Protection Agency [US EPA] Integrated Risk Information System [IRIS], 2005)

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- *Screening*:
  - 6.7B-Suspected human carcinogens (New Zealand-Globally Harmonized System [GHS])
  - Carcinogenicity Category 2 (Japan)

National Toxicology Program (NTP) (2004, as cited in Organisation for Economic Co-operation and Development [OECD], 2012)

- NTP (2004, as cited in OECD, 2012) conducted two bioassays, one in mice and another in rats, on the surrogate solvent naphtha, (petroleum), medium aliphatic, composed of primarily C10-13 aliphatic hydrocarbons with < 1% aromatic hydrocarbons (CAS# 64742-88-7). The study summary results are described below.
  - A two year carcinogenicity study conducted by the NTP was identified in which the surrogate, solvent naphtha, (petroleum), medium aliphatic (CAS# 64742-88-7), was administered *via* inhalation at concentrations of 0, 138, 550, and 1,100 mg/mg^3 for male F344/N rats and 550, 1,100, and 2,200 mg/mg^3 for female F344/N rats. In male rats, increased incidences of renal tubule hyperplasia (a preneoplastic lesion) were observed at 550 mg/m^3 and 1,100 mg/m^3. The incidence of renal tubule adenoma was increased in 1,100 mg/m^3 for males, however, it was not statically significant compared to the controls. In the adrenal medulla, the incidences of benign adrenal pheochromocytomas were significantly increased in males at 550 mg/m^3 and 1,100 mg/m^3. The incidences of malignant adrenal pheochromocytomas were significantly increased in males at 1,100 mg/m^3. However, pheochromocytomas are frequently observed in studies of F344/N rats and are reported to be of questionable relevance to humans (Greim *et al*., 2009). There was no evidence of carcinogenicity in female rats at any exposure concentration tested (NTP, 2004, as reported in OECD, 2012).
  - A second NTP study exposed B6C3F1 mice to 0, 550, 1,100, or 2,200 mg/m^3 to the surrogate, solvent naphtha, (petroleum), medium aliphatic, composed of primarily C10-13 aliphatic with < 1% aromatic (CAS# 64742-88-7). There was increased incidence of hepatocellular adenoma in males at 2,200 mg/m^3, however, it was not statistically significant compared to the controls. Evidence was equivocal for the increase in hepatocellular adenoma incidence in female mice at 2,200 mg/m^3 (18/50 compared to controls 9/50, $p = 0.032$), as the increase was viewed by NTP as a consequence of increased body weight (NTP, 2004, as reported in OECD, 2012).

Summary

ECOSOLV is assigned a score of *Moderate (M)* for carcinogenicity *via* the oral route of exposure based on the surrogate's presence on authoritative lists under potential residual hazards (or impurities). Note that a GHS weight-of-evidence evaluation indicates equivocal results from two carcinogenicity studies (one in rats, one in mice) conducted with a surrogate. Because the available information is for a surrogate and not for ECOSOLV itself, a low confidence is assigned to this score.

Solvent naphtha, (petroleum), medium aliphatic, composed of primarily C10-13 aliphatic with < 1% aromatic (CAS# 64742-88-7) was selected by Gradient chemists as a surrogate due to the availability of carcinogenicity data and its similarity to ECOSOLV in terms of functional groups and physical and chemical properties. The surrogate is made up of linear, branched, and/or cyclic paraffins in the C10 to C13 range. There is equivocal evidence that surrogate solvent naphtha, (petroleum), medium aliphatic,

composed of primarily C10-13 aliphatic with < 1% aromatic (CAS# 64742-88-7) is carcinogenic in rats and mice. National Toxicology Program (NTP) concluded that while there was some evidence of carcinogenicity in male rats based on the adrenal tumors, although it should also be noted that the observed tumors, pheochromocytomas, are a common spontaneous tumor in F344 rats but are rare in humans. NTP also concluded that while there was some increased incidence of hepatocellular adenoma in female mice, the effects seen may be a consequence of increased body weight.

ECOSOLV and the surrogate (CAS# 64742-88-7) used are not listed by any GreenScreen-specified list as carcinogens. However, under the potential residual hazard section, the surrogate is listed by both authoritative (MAK Group 4 classification and IARC 2B classification) and screening (Category 2 assignments from Japan and New Zealand (converted from 6.7B) GreenScreen lists as a potential carcinogen. These classifications translate to a moderate hazard assignment for this endpoint. Under the same potential residual hazard section, the surrogate is also listed on an authoritative list (CalEPA Proposition 65) as a carcinogen, which would translate to a high (H) score. However, this classification is based on an impurity, ethylbenzene, which we have not been able to confirm as being present in ECOSOLV. If additional information on the impurities in ECOSOLV becomes available, this endpoint should be re-evaluated.

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

ECOSOLV is assigned a score of **Low (L)** for mutagenicity/genotoxicity based on a demonstrated lack of mutagenic or genotoxic effects in *in vitro* and *in vivo* studies of suitable surrogates. While no data were identified for ECOSOLV itself, a high confidence is assigned due to the available data for the surrogates and high data quality (OECD studies).

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed
- *Screening*: Not listed

In vitro Assays

OECD (2012)

- C10-C12 isoalkanes (CAS# 90622-57-4) was not mutagenic in *Salmonella* strains tested in Bacterial Reverse Mutation assays (OECD TG 471), with or without metabolic activation.
- C10-C12 isoalkanes (CAS# 90622-57-4) did not induce any mutations in a Sister Chromatid Exchange assay in mammalian cell lines (OECD TG 479).

In vivo Assays

OECD (2012)

- Solvent naphtha, (petroleum), medium aliphatic, composed of primarily C10-13 aliphatic (CAS# 64742-88-7) was not genotoxic *via* inhalation exposure in a Micronucleus Assay in mouse bone marrow (OECD TG 474).

- C10-C12 isoalkanes (CAS# 90622-57-4) was not genotoxic *via* inhalation exposure in a Rodent Dominant Lethal Test (OECD TG 478).

Summary

ECOSOLV is assigned a score of **Low (L)** for mutagenicity/genotoxicity based on a demonstrated lack of mutagenic or genotoxic effects in several *in vitro* and *in vivo* OECD guidelines studies involving the selected suitable surrogates. While no data were identified for ECOSOLV itself, a high confidence is assigned to this score due to the data available for the strong surrogate and high data quality (OECD studies).

Solvent naphtha, (petroleum), medium aliphatic, composed of primarily C10-13 aliphatic (CAS# 64742-88-7) and C10-C12 isoalkanes (CAS# 90622-57-4) were selected by Gradient chemists as an appropriate surrogates for ECOSOLV due to the availability of mutagenicity data and similarity to ECOSOLV in terms of functional groups and physical and chemical properties. The surrogates are made up of linear, branched, and/or cyclic paraffins in C10 to C13 range. The compounds were not mutagenic in *in vitro* assays including bacterial reverse mutation assays and sister chromatid exchange assays. They were also not genotoxic in OECD guideline mouse bone marrow micronucleus assays and a rodent dominant lethal test, both following inhalation exposure.

ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as mutagens.

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

ECOSOLV is assigned a *Low (L)* score for reproductive toxicity based on the limited details in a single surrogate study. Confidence in the assignment is low because the study was limited in details and there are no studies for ECOSOLV on this endpoint. ECOSOLV and its surrogates were not listed on any GreenScreen lists for this endpoint.

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed
- *Screening*: Not listed

Cosmetic Ingredient Review (CIR) Expert Panel (2010) and Johnson *et al.* (2012)

In a combined subchronic and reproductive toxicity study, Sprague Dawley rats (20 male and 20 females/group) were exposed to 0, 200 parts per million (ppm) (1,400 mg/m^3 or 1.4 mg/L), 600 ppm (4,200 mg/m^3 or 4.2 mg/L), or 1,800 ppm (123,600 mg/m^3 or 123.6 mg/L) of isododecane (CAS# 141-70-8) 6 days per week for 13 weeks. At 600 ppm (4,200 mg/m^3 or 4.2 mg/L) and above, increases in kidney weights and respiratory tract inflammation were observed. At 1,800 ppm (123,600 mg/m^3 or 123.6 mg/L), an increase in incidence of tubular nephrosis in male rats was observed. At 1,800 ppm (123,600 mg/m^3 or 123.6 mg/L), increased relative weights in gonads in males were observed. The study authors did not opine on the clinical significance of increased gonad weight or the absolute weight increase.

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Summary

ECOSOLV is assigned a *Low (L)* score for reproductive toxicity based on the limited details in a single surrogate study reporting increased relative gonad weight of unknown clinical significance in males. Confidence in this score is low because the study was limited in details and there are no studies specifically for ECOSOLV on this endpoint.

Isododecane (CAS# 141-70-8) was selected by Gradient chemists as a surrogate due to the availability of reproductive toxicity data and its similarity to ECOSOLV in terms of functional groups and physical and chemical properties. The surrogate is a mixture of branched C12 alkanes.

The study reviewed indicated there was increased relative gonad weight of unknown clinical significance in males, however, the effect was observed only at a dose of 1,800 ppm (123,600 mg/m^3 or 123.6 mg/L) that was already demonstrated to be toxic to the parental animals. At 600 ppm (4200 mg/m^3 or 4.2 mg/L) and above, increases in kidney weights and respiratory tract inflammation were observed. At 1,800 ppm (123,600 mg/m^3 or 123.6 mg/L), increases in the incidence of tubular nephrosis in male rats were observed. Under GHS, clear reproductive effects would include those clinically significant and only observed at levels that do not produce significant systemic toxicity to the parental animals (*i.e.*, to ensure that reproductive effects are not due to secondary non-specific consequences to other toxic effects).

ECOSOLV and the surrogate isododecane were not listed on any GreenScreen lists for this endpoint.

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

ECOSOLV is assigned a *Low (L)* score for developmental toxicity based on the limited details in a single surrogate study reporting no fetotoxicity or teratogenicity following inhalation exposure up to 900 ppm on gestational days 6 to 15. Confidence in the assignment is low because the study was limited in details and there are no studies using ECOSOLV for this endpoint.

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed
- *Screening*: Not listed

CIR Expert Panel (2010) and Johnson *et al.* (2012)

- In a developmental toxicity study, pregnant Sprague Dawley rats were exposed to 0, 300, or 900 ppm of Isopar® G, a C10-11 isoparaffin (CAS# 246538-75-0) 6 hours per week on gestational days 6 to 15. The number of rats per dose group was not included in the unpublished data (as cited in Johnson *et al*., 2012). At gestational day 21, the dams were sacrificed and fetuses were evaluated for developmental effects. No malformations (external, visceral, or skeletal) or effects on resorptions, fetal size, and sex distribution were observed in the fetuses.

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Summary

ECOSOLV is assigned a *Low (L)* score for developmental toxicity based on the limited details in a single surrogate study reporting no fetotoxicity or teratogenicity following inhalation exposure up to 900 ppm on gestational days 6 to 15. None of the observed parameters indicated there were developmental effects.

Isopar G, a C10-11 isoparaffin, was selected by Gradient chemists as an appropriate surrogate due to the availability of developmental toxicity data and its similarity to ECOSOLV in terms of functional groups and physical and chemical properties. The surrogate is a mixture of branched C10-11 alkanes. Confidence in the assignment is low because the study was limited in details and there are no studies for ECOSOLV on this endpoint. ECOSOLV and surrogate were not listed on any GreenScreen lists for this endpoint.

Endocrine Activity (E) Score (H, M, or L): dg

ECOSOLV is assigned a data gap (dg) for endocrine activity. ECOSOLV and its surrogates were not listed on any GreenScreen lists for this endpoint.

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed
- *Screening*: Not listed

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

Note: *Group II and Group II* endpoints are distinguished in the v 1.3 Benchmark system (the asterisk indicates repeated exposure). For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints. When classifying hazard for Systemic Toxicity/Organ Effects and Neurotoxicity endpoints, repeated exposure results are required and preferred. Lacking repeated exposure results in a data gap. Lacking single exposure data does not result in a data gap when repeated exposure data are present (shade out the cell in the hazard table and make a note). If data are available for both single and repeated exposures, then the more conservative value is used.*

Acute Mammalian Toxicity (AT) Group II Score (vH, H, M, or L): L

ECOSOLV is assigned a score of **Low (L***)* for acute oral, dermal, and inhalation mammalian toxicity. The level of confidence in this score is high because all studies using ECOSOLV and the surrogate(s) used for this endpoint showed low acute toxicity following oral, dermal, and inhalation exposure. Additionally, ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as an acute mammalian toxicant.

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed

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- *Screening*: Not listed

Studies

Table 5 Acute Oral Toxicity Studies

Name	Chain Length	CAS#	LD_{50}	Species	Study Method	Reference
ECOSOLV	C12-C14	68551-19-9	> 3,900 mg/kg-bw	Rat	Not Reported	Chevron, 2013
Isopar® G	C10-11	246538-75-0	> 10,000 mg/kg-bw	Rat	Not Reported	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Isopar® L	C11-13	246538-78-3	> 10,000 mg/kg-bw	Rat	Not Reported	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Soltrol® 130	C10-C13	68551-17-7	> 34,600 mg/kg-bw	Rat	Not Reported	CIR Expert Panel, 2010 and Johnson *et al.*, 2012

Notes:
CAS = Chemistry Abstracts Service; LD_{50} = Median Lethal Dose.

Table 6 Acute Dermal Toxicity Studies

Name	Chain Length	CAS#	LD_{50}	Species	Study Method	Reference
ECOSOLV	C12-C14	68551-19-9	> 2,000 mg/kg-bw	Rabbit	Not Reported	Chevron, 2013
Isopar® G	C10-11	246538-75-0	> 3,200 mg/kg-bw	Rabbit	Not Reported	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Isopar® L	C11-13	246538-78-3	> 3,200 mg/kg-bw	Rabbit	Not Reported	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Soltrol® 130	C10-C13	68551-17-7	-15,400 mg/kg-bw [sic]	Rabbit	Not Reported	CIR Expert Panel, 2010 and Johnson *et al.*, 2012

Notes:
CAS = Chemistry Abstracts Service; LD_{50} = Median Lethal Dose.

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Table 7 Acute Inhalation Toxicity Studies

Name	Chain Length	CAS#	LC_{50}	Duration	Physical State	Species	Study Method	Reference
ECOSOLV	C12-C14	68551-19-9	> 5.3 mg/L	4 Hours	Dust/ Mist	Rat	Not Reported	Chevron, 2013
Isopar® G	C10-11	246538-75-0	> 12.2 mg/L	4 Hours	Not Reported	Rat	Not Reported	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Isopar® L	C11-13	246538-78-3	> 5.01 mg/L	4 Hours	Not Reported	Rat	Not Reported	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Soltrol® 130	C10-C13	68551-17-7	> 8.2 mg/L	6 Hours	Not Reported	Rat	Not Reported	CIR Expert Panel, 2010 and Johnson *et al.*, 2012

Notes:
CAS = Chemistry Abstracts Service; LC_{50} = Median Lethal Concentration.

Summary

ECOSOLV is assigned a score of **Low (L***)* for acute oral, dermal, and inhalation mammalian toxicity. The level of confidence in this score is high because all of the studies on ECOSOLV and the surrogate(s) used for this endpoint demonstrated low acute toxicity following oral, dermal, and inhalation exposure (Tables 5 through 7).

Acute toxicity data located for ECOSOLV under a Chevron SDS for Soltrol® 170 did not capture the LD_{50} or LC_{50} at the levels tested. In other words, the LD_{50} or LC_{50} must be higher than the dose tested because less than 50% of the test animals died at the concentrations tested. Thus, studies using other isoparaffins of similar chain length were also used to inform this endpoint. The surrogates selected by Gradient's chemists included Isopar® G C10-11, Isopar® L C11-13, and Soltrol® 130 C10-C13 due to the availability of acute toxicity data and their similarity to ECOSOLV in terms of functional groups and physical and chemical properties; these surrogates are all branched isoparaffins in the C10 to C13 range. The studies for these surrogates studies also did not report any true LD_{50} or LC_{50} at the levels tested because less than 50% of animals died at those concentrations, providing additional support for assigning the **Low (L)** score.

ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as an acute mammalian toxicant.

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Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)

(ST-Single) Group II Score (vH, H, M, or L): dg

ECOSOLV is assigned a data gap (dg) for single exposure systemic toxicity/organ effects. While acute toxicities studies were located for ECOSOLV and several surrogates (isoparaffins in C10 to C13 range), no clinical details were reported on those studies.

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed
- *Screening*: Not listed

(ST-Repeated) Group II* Score (H, M, L): *L*

ECOSOLV is assigned a *Low (L)* score for systemic toxicity *via* repeated inhalation exposure based on a surrogate study reporting effects observed only at high dosages that well exceed the GHS and GreenScreen criteria for hazard classification for this endpoint. Confidence in this score is low because the study was limited in details and there were no studies identified specifically for ECOSOLV on this endpoint. ECOSOLV and the surrogate were not listed on any GreenScreen lists for this endpoint.

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed
- *Screening*: Not listed

CIR (2010)

- In a combined subchronic and reproductive toxicity study, Sprague Dawley rats (20 male and 20 females/group) were exposed to 0, 200 ppm (1,400 mg/m^3 or 1.4 mg/L), 600 ppm (42,00 mg/m^3 or 4.2 mg/L), or 1,800 ppm (123,600 mg/m^3 or 123.6 mg/L) of Isododecane (CAS# 141-70-8) 6 days per week for 13 weeks. At 600 ppm (4,200 mg/m^3 or 4.2 mg/L) and above, increases in kidney weights and respiratory tract inflammation were observed. At 1,800 ppm (123,600 mg/m^3 or 123.6 mg/L), increases in incidence of tubular nephrosis and relative gonad weights in male rats were observed. The study authors did not opine on the significance of the clinical effects observed.

Summary

ECOSOLV is assigned a *Low (L)* score for systemic toxicity *via* repeated inhalation exposure based on a surrogate study reporting effects observed only at high dosages that well exceed the GHS and

GreenScreen criteria for classification under this endpoint. Confidence in the score is low because the study was limited in details and there are no studies for ECOSOLV on this endpoint.

Due to the lack of data for ECOSOLV, surrogate data were reviewed to inform this endpoint. Isododecane (CAS# 141-70-8), a branched C12 isoparaffin, was selected by Gradient chemists as an appropriate surrogate for ECOSOLV due to the availability of repeated toxicity data and its similarity to ECOSOLV in terms of functional groups and physical and chemical properties.

In a 13 week inhalation study in rats, increases in kidney weight and respiratory tract inflammation were observed at 600 ppm (4,200 mg/m^3 or 4.2 mg/L) and 1,800 ppm (123,600 mg/m^3 or 123.6 mg/L) following exposure to the surrogate isododecane (CAS# 141-70-8). At 1,800 ppm (123,600 mg/m^3 or 123.6 mg/L), increased incidence of tubular nephrosis and relative gonad weights in male rats were also observed. While the study authors did not opine on the clinical significance of the effects observed, these effects were observed only at high dosages that well exceed GHS and GreenScreen criteria of classification on this endpoint. Under GHS, maximum classifiable lowest observed adverse effect level (LOAEL) under this endpoint is 0.2 mg/L (mist) or 1.0 mg/L (vapor) for inhalation exposure. At the lowest dose tested, 200 ppm (1,400 mg/m^3 or 1.4 mg/L), no clinical effects were observe in rats. The study authors did not report whether the test substance was administered *via* vapor or mist. Nonetheless, the no observed adverse effect level (NOAEL) of 200 ppm (1,400 mg/m^3 or 1.4 mg/L) is also above the GHS and GreenScreen classification cut off for this endpoint (> 1 mg/L for vapor and > 0.2 mg/L for mist).

ECOSOLV and the surrogate were not listed on any GreenScreen lists for this endpoint.

Neurotoxicity (N)

Neurotoxicity (N) Group II Score (Single Exposure: vH, H, M, or L): *M*

ECOSOLV is assigned a score of *Moderate (M)* for neurotoxicity – single exposure, based on two studies of surrogate neurotoxicity studies. Confidence in this score is low because the surrogate studies were limited in details and there are no studies specifically using ECOSOLV for this endpoint. ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as neurotoxicants.

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed
- *Screening*: Not listed

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Table 8 Neurotoxicity Animal Studies

Chemical	CAS#	Species	Dose	Study Detail	Duration	Results	Reference
C11-C12 Isoalkane, < 2% Aromatics[a]	None Given	Male Mouse	500, 1,000, 2,000, 4,000 ppm Vapor (locomotive activity not examined at 4,000 ppm)	1997, Klimisch Score 1	2 Days per Week for Unknown Weeks	Locomotive and Operant Parameter: NOAEC ≥ 2,000 ppm (11,600 mg/m^3); at 4,000 ppm, Slower Response Rate for Operant Test Observed	ECHA, 2016a
C10-C12 Isoalkane, < 2% Aromatics	None Given	Rat	0, 85 ppm (500 mg/m^3), 260 ppm (1,500 mg/m^3), 860 ppm (5,000 mg/m^3) Vapor	2001, Klimisch Score 2	3 Days	Learned Performance Parameter: NOAEC > 260 ppm (1,500 mg/m^3); at 860 ppm (5,000 mg/m^3) Mild Effects on Performance Speed Observed	ECHA, 2016a

Notes:
CAS = Chemistry Abstracts Service; NOAEC = No Observed Adverse Effect Concentration.
(a) C7-C8, C8-C9, C10-C11 isoalkane were also tested in this study. However, their results are not reported because C11-C12 is the strongest surrogate for ECOSOLV based on chain length.

Summary

ECOSOLV is assigned a score of *Moderate (M)* for neurotoxicity based on two studies of surrogate neurotoxicity studies (Table 8). Confidence is low in this score because the surrogate studies were limited in details and there are no studies specifically using ECOSOLV for this endpoint.

Based on acute exposure, mild effects on cognitive functions and response rates were observed in rodents following inhalation exposure to C11-C12 isoalkane and C10-C12 isoalkane at high dosages. Since the effects are mild and do not appear to indicate a significant alteration of nervous system structure or function and are likely transient in nature, a GreenScreen assignment of Moderate is assigned. C11-C12 isoalkane, < 2% aromatics and C10-C12 isoalkane, < 2% aromatics were selected by Gradient chemists as appropriate surrogates due to the availability of neurotoxicity data and their similarity to ECOSOLV in terms of functional groups and physical and chemical properties.

ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as a neurotoxicant.

Neurotoxicity (N) Group II* Score (Repeated Exposure: H, M, or L): dg

ECOSOLV is assigned a data gap (dg) for neurotoxicity – repeated exposure. ECOSOLV and the surrogate were not listed on any GreenScreen lists for this endpoint.

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

ECOSOLV is assigned a score of *Low (L)* for skin sensitization based on lack of sensitization observed in animal and human studies of other isoparaffins of similar chain length. There is low confidence in this

score because no studies were identified specifically for ECOSOLV and the surrogate studies reviewed are limited in study details. ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as a dermal sensitizer.

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed
- *Screening*: Not listed

Table 9 Skin Sensitization Animal Studies

Name	Chain Length	CAS#	N	Concentration	Study Method	Effects	Reference
Isopar® L	C11-13	246538-78-3	Not Reported	Not Reported	Guinea Pig Maximization	No Evidence of Skin Sensitization	CIR Expert Panel, 2010 and Johnson *et al.*, 2012

Notes:
CAS = Chemistry Abstracts Service; N = Number (of animals).

Table 10 Skin Sensitization Human Studies

Name	Chain Length	CAS#	N	Concentration	Study Method	Effects	Reference
Isopar® G	C10-11	246538-75-0	> 100	50% in Petrolatum	Patch (semi-occlusive)	No Evidence of Skin Sensitization	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Isopar® L	C11-13	246538-78-3	> 100	50% in Petrolatum	Patch (semi-occlusive)	No Evidence of Skin Sensitization	CIR Expert Panel, 2010 and Johnson *et al.*, 2012

Notes:
CAS = Chemistry Abstracts Service; N = Number (of animals).

Summary

ECOSOLV is assigned a score of *Low (L)* for skin sensitization based on lack of sensitization observed in studies of other isoparaffins of similar chain length (Tables 9 and 10). In both the guinea pig maximization and human patch test studies we reviewed, no evidence of dermal sensitization was observed when isoparaffins of similar chain length were applied to the skin (Johnson *et al*., 2012; ECHA, 2015). Isopar® L and Isopar® G were selected by Gradient chemists as appropriate surrogates due to the availability of sensitization data and their similarity to ECOSOLV in terms of functional groups and physical and chemical properties. The surrogates are all branched isoparaffins in the C10 to C13 range. There is low confidence in this score because no studies were located on ECOSOLV and the surrogate studies reported are limited in study details.

ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as a dermal sensitizer.

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

ECOSOLV was assigned a data gap (dg) for respiratory sensitization because no relevant data were identified for this endpoint for ECOSOLV or its surrogates. ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as a respiratory sensitizer.

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

ECOSOLV is assigned a score of *High (H)* for skin irritation based on animal studies for surrogates where moderate to severe irritation was observed. This translated into a GHS classification as a Category 2 skin irritant. There is low confidence in this score because no studies were identified specifically for ECOSOLV and the surrogate studies we reviewed are limited in study details. ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as a dermal irritant.

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed
- *Screening*: Not listed

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Studies

Table 11 Skin Irritation Animal Studies

Name	Chain Length	CAS#	Animal	Concentration	Study Method	Effects	Reference
Isopar® G	C10-11	246538-75-0	Rabbit	Not Reported	24 Hour Application	Slight Dose-related Irritation	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Isopar® G	C10-11	246538-75-0	Rabbit	Undiluted	Modified Non-occlusive Patch Test	Non-irritant	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Isopar® G	C10-11	246538-75-0	Rabbit	Undiluted	Occlusive Patch Test	Primary Irritation (grade 5)	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Isopar® L	C11-13	246538-78-3	Rabbit	Not Reported	Not Reported	Slight Skin Irritation	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Soltrol® 130	C10-13	68551-17-7	Rabbit	Not Reported	Draize	Primary Irritation (grade 5.7)	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Soltrol® 130	C10-13	68551-17-7	Rabbit	Not Reported	Application to Intact or Abraded Skin	Very Slight to Severe Irritation	CIR Expert Panel, 2010 and Johnson *et al.*, 2012

Note:
CAS = Chemistry Abstracts Service.

Summary

ECOSOLV is assigned a score of *High (H)* for skin irritation based on moderate to severe irritation observed in animal studies involving surrogates (Table 11) as well as the inherent potential of paraffins causing irritation through defatting. There is low confidence in this score because no studies were identified specifically for ECOSOLV and the studies reviewed for the surrogates provided limited details.

No study data were located specifically for ECOSOLV on this endpoint, thus isoparaffins of similar chain length were selected as surrogates. Isopar® L, Isopar® G, and Soltrol® 130 were selected by Gradient chemists as appropriate surrogates due to the availability of skin irritation data and their similarity to ECOSOLV in terms of functional groups and physical and chemical properties. These surrogates are all branched isoparaffins in the C10 to C13 range.

According to Johnson *et al*. (2012), isoparaffins and normal paraffins can produce defatting of the skin and subsequent irritation, if application of test substance is under closed or semi-occlusive conditions where evaporation cannot freely occur. The surrogate animal studies we reviewed reported a range of results, from no irritation under a modified non-occlusive patch test of undiluted test substance, to moderately to severely irritating (grades 5-6) in rabbits under occlusive patch tests of another undiluted test substance. Primary skin irritation scores between 5 and 6 are considered to be moderately to severely irritating. The range of different irritative results is likely attributed to the different study methods and reporting criteria employed. Based on GHS criteria, this would translate into a Category 2 skin irritant.

ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as a dermal irritant.

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

ECOSOLV is assigned a score of *Moderate (M)* for eye irritation/corrosivity based on minimal eye irritation observed in animal studies involving surrogates. This translated into a GHS classification as a Category 2B eye irritant. There is low confidence in this score because no studies were identified specifically for ECOSOLV and the studies involving surrogates provided limited details. ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as an eye irritant.

Authoritative and Screening Lists

ECOSOLV and surrogate(s) used for this endpoint

- *Authoritative*: Not listed
- *Screening*: Not listed

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Studies

Table 12 Eye Irritation Animal Studies

Name	Chain Length	CAS#	Animal	Concentration	Study Method	Effects	Reference
Isopar® G	C10-11	246538-75-0	Rabbit	Not Reported	Draize	No Effects Draize Score of 0 to 1 Out of 110 Max Score	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Isopar® L	C11-13	246538-78-3	Rabbit	Not Reported	Draize	Draize Score of 0 to 6 Out of 110 Max Score Slight Conjunctival Irritation, but No Corneal Lesions	CIR Expert Panel, 2010 and Johnson *et al.*, 2012
Soltrol® 130	C10-13	68551-17-7	Rabbit	Not Reported	Not Reported	Conjunctival Redness and Discharge Grade 1 (presumably out of 4), but No Corneal Opacity	CIR Expert Panel, 2010 and Johnson *et al.*, 2012

Note:
CAS = Chemistry Abstracts Service.

Summary

ECOSOLV is assigned a score of *Moderate (M)* for eye irritation/corrosivity based on minimal eye irritation observed in animal studies involving surrogates (Table 12). There is low confidence in this score because no studies were identified specifically for ECOSOLV and the surrogate studies we reviewed provided limited details.

As no data were identified specifically for ECOSOLV on this endpoint, isoparaffins of similar chain length were used as surrogates. Isopar® L, Isopar® G, and Soltrol® 130 were selected by Gradient chemists as appropriate surrogates due to the availability of eye irritation data and similarity to ECOSOLV in terms of functional groups and physical and chemical properties. The surrogates are all branched isoparaffins in C10 to C13 range.

The surrogate studies we reviewed reported no to mild eye irritation in rabbits. In the two Draize studies, surrogate Isopar® G, scored a maximum 1 out of 110 indicating that the substance is practically non-irritating to the eyes. Isopar® L, scored a maximum 6 out of 110, indicating that the substance is minimally irritating. Another surrogate, Soltrol® 130, reported grade 1 (presumably out of 4) indicating minimal irritation as well. No human studies were available for the surrogates we evaluated.

ECOSOLV and the surrogates used to inform this endpoint are not listed by any GreenScreen-specified list as an eye irritant.

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Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): *L*

ECOSOLV is assigned a score of *Low* (*L*) for acute aquatic toxicity based on the results of multiple aquatic toxicity studies for two suitable surrogates (summarized below in Table 13). Surrogates were selected due to their similarity to ECOSOLV in terms of functional groups and physical and chemical properties. These surrogates are made up of linear, branched, and/or cyclic paraffins in the C9 to C13 range. No acute aquatic toxicity data were identified for ECOSOLV itself, nor was it present on any authoritative or screening lists. Measured toxicity data were identified for two strong surrogates, indicating low acute aquatic toxicity. Three additional suitable surrogates were present on a screening list, indicating inherent toxicity, which would translate to a score of very high for acute aquatic toxicity. Therefore, low confidence is assigned to the acute aquatic toxicity score for ECOSOLV because of the conflicting assignments between the surrogate data and screening lists, and because only surrogate experimental data were available.

Authoritative and Screening Lists

ECOSOLV

- *Authoritative*: Not listed
- *Screening*: Not listed

Solvent naphtha (petroleum), medium aliphatic (CAS# 64742-88-7), C10-13 Isoparaffin (CAS# 68551-17-7), and 2,2,4,6,6-Pentamethylheptane (CAS# 13475-82-6)

- *Authoritative*: Not listed
- *Screening*:
    - Environment Canada (EC) – Canadian Environmental Protection Act (CEPA) Domestic Substances List (DSL) - Inherently Toxic in the Environment

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Table 13 Acute Ecotoxicity Data for ECOSOLV Surrogates

Trophic Level	Test Species	Endpoint	Value (mg/L)[a]	Method	Source
Test material: Hydrocarbons, C10-C12, Containing Isoalkanes with Less than 2% Aromatics (no CAS#)					
Fish	Rainbow Trout (*Oncorhynchus mykiss*)	96 Hour LL_{50}	> 1,000	OECD TG 203	ECHA, 2015
Invertebrate	Water Flea (*Daphnia magna*)	48 Hour EL_{50}	> 1,000	OECD TG 202	
Invertebrate	Marine Amphipod (*Chaetogammarus marinus*)	96 Hour LL_{50}	> 1,000	US EPA OPPTS 850.1020	
Algae	Green Algae (*Pseudokirchneriella subcapitata*)	72 Hour EL_{50}	> 1,000	OECD TG 201	
Test material: C9-12 Isoparaffin (CAS# 90622-57-4)					
Fish	Fathead Minnow (*Pimephales promelas*)	96 Hour LC_{50}	2,600- > 5,000	OECD TG 203	EC, ECB, 2000b

Notes:
CAS = Chemistry Abstracts Service; EL_{50} = Median Effect Loading Rate; LC_{50} = Median Lethal Concentration; LL_{50} = Median Lethal Loading Rate.
(a) Nominal concentration unless otherwise noted.

Due to a lack of acute aquatic toxicity data for ECOSOLV, surrogate data were used to assign an acute aquatic toxicity score. Table 13 presents a summary of fish, invertebrate, and algae acute aquatic toxicity data for two suitable surrogates of ECOSOLV. These data were all generated following regulatory (OECD, EPA) guideline methods. Nominal Median Loading Rate Effect (EL_{50}) and Median Lethal Loading Rate/Concentration (LL/C_{50}) values above 100 mg/L indicate that ECOSOLV exhibits low acute aquatic toxicity in accordance with the GreenScreen guidance for the acute aquatic toxicity endpoint. However, because three other surrogates of ECOSOLV were present on a screening list indicating very high acute aquatic toxicity according to GreenScreen guidance, and because the available experimental data are for surrogates only, the score was assigned low confidence.

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): *vH*

ECOSOLV is assigned a score of *Very High* (*vH*) for chronic aquatic toxicity based on the results of chronic aquatic toxicity studies for suitable surrogates (summarized below in Table 14) and the presence of other suitable surrogates on a screening list. Surrogates were selected due to their similarity to ECOSOLV in terms of functional groups and physical and chemical properties. These surrogates are made up of linear, branched, and/or cyclic paraffins in the C9 to C13 range. No chronic aquatic toxicity data were identified for ECOSOLV itself, nor was it present on any authoritative or screening lists. The chronic aquatic toxicity score is assigned low confidence because of the quality of the surrogate data and because none of the surrogates were present on authoritative lists.

Authoritative and Screening Lists

ECOSOLV

- *Authoritative*: Not listed
- *Screening*: Not listed

Solvent naphtha (petroleum), medium aliphatic (CAS# 64742-88-7), C10-13 Isoparaffin (CAS# 68551-17-7), and 2,2,4,6,6-Pentamethylheptane (CAS# 13475-82-6)

- *Authoritative*: Not listed
- *Screening*:
  - EC - CEPA DSL - Inherently Toxic in the Environment

Table 14 Chronic Aquatic Toxicity Data for ECOSOLV Surrogates

Trophic Level	Test Species	Endpoint	Value (mg/L)[a]	Method	Source
Test material: Hydrocarbons, C10-C12, Containing Isoalkanes with Less than 2% Aromatics (no CAS#)					
Fish	Rainbow Trout (*Oncorhynchus mykiss*)	28 Day NOELR	0.192	Petrotox Model	ECHA, 2016b
Invertebrate	Water Flea (*Daphnia magna*)	21 Day NOELR	< 1	OECD TG 211	
Test material: C9-12 Isoparaffin (CAS# 90622-57-4)					
Invertebrate	Water Flea (*Daphnia magna*)	Chronic NOEC	0.025 (measured)	NR	OECD, 2012

Notes:
CAS = Chemistry Abstracts Service; NOEC = No Observed Effect Concentration; NOELR = No Observed Effect Loading Rate; NR = Not Reported.
(a) Nominal measured concentration unless otherwise noted.

Surrogate data were used to assign a chronic aquatic toxicity score, due to a lack of chronic aquatic toxicity data for ECOSOLV. Table 14 presents a summary of fish and invertebrate chronic aquatic toxicity data for two surrogates of ECOSOLV. No Observed Effect Concentration (NOEC) or Loading Rate (NOELR) values below 0.1 mg/L indicate that ECOSOLV exhibits very high chronic aquatic toxicity in accordance with the GreenScreen guidance for the chronic aquatic toxicity category. Three other surrogates were present on a screening list, indicating very high chronic aquatic toxicity. However, because all of the available experimental data are for surrogates, the test method was only reported for one of the values, and because another of the values was generated from a model, the chronic aquatic toxicity score is assigned with low confidence.

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): *H*

ECOSOLV is assigned a score of *High* (*H*) for persistence based on the results of percent biodegradation studies for suitable surrogates (summarized below in Table 15). Surrogates were selected due to their similarity to ECOSOLV in terms of functional groups and physical and chemical properties. These surrogates are made up of linear, branched, and/or cyclic paraffins in the C9 to C12 range. No persistence data were identified for ECOSOLV itself, nor was it present on any authoritative or screening lists. Although the surrogate data are of high quality, the persistence score is assigned low confidence since it is based on biodegradation, not half-life, data.

Authoritative and Screening Lists

ECOSOLV and Surrogates

- *Authoritative*: Not listed
- *Screening*: Not listed

Table 15 Degradation Data for ECOSOLV Surrogates

Test Medium	Endpoint (units)	Value	Method	Source
Test material: Hydrocarbons, C10-C12, Containing Isoalkanes with Less Than 2% Aromatics (no CAS#)				
Activated sludge, domestic	28 Day % Degradation	31-41.7	OECD TG 301F	ECHA, 2016b
Test material: C9-12 Isoparaffin (CAS# 90622-57-4)				
Domestic sewage, non-adapted	28 Day % Degradation	21.9	OECD TG 301F	EC, ECB, 2000b
Test material: Solvent Naphtha (petroleum), Medium Aliphatic (CAS# 64742-88-7)				
Domestic sewage	25 Day % Degradation	57	OECD TG 301B	EC, ECB, 2000c

Note:
CAS = Chemistry Abstracts Service.

Surrogate data were used to assign a persistence score, due to a lack of persistence data for ECOSOLV. Table 15 presents a summary of available biodegradation data for three ECOSOLV surrogates. The measured surrogate biodegradation data indicate that ECOSOLV is inherently, but not rapidly, biodegradable. Therefore, a conservative persistence score of high was assigned to ECOSOLV. The score is assigned with low confidence because it is not based on half-life data and because only surrogate data were available.

Bioaccumulation (B) Score (vH, H, M, L, or vL): vH

ECOSOLV is assigned a score of **Very High** (**vH**) for bioaccumulation based on the partition coefficient (Log K_{ow}) and bioconcentration factor (BCF) values for suitable surrogates (summarized below in Table 16) and the presence of one of ECOSOLV's surrogates on a screening list. Surrogates were selected due to their similarity to ECOSOLV in terms of functional groups and physical and chemical properties. These surrogates are made up of linear, branched, and/or cyclic paraffins in the C9 to C12 range. No bioaccumulation data were identified for ECOSOLV itself, nor was it present on any authoritative or screening lists. The surrogate data and the screening list all indicate that ECOSOLV's bioaccumulative potential score is very high, so the score is assigned high confidence.

Authoritative and Screening Lists

ECOSOLV

- *Authoritative*: Not listed
- *Screening*: Not listed

Solvent naphtha (petroleum), medium aliphatic (CAS# 64742-88-7)

- *Authoritative*: Not listed
- *Screening*:

- EC - CEPA DSL - Bioaccumulative

Table 16 Bioaccumulation Data for ECOSOLV Surrogates

Parameter	Test Species	Endpoint	Value	Method	Source
Test material: 2,2,4,6,6-Pentamethylheptane (CAS# 13475-82-6)					
Octanol-water Partition Coefficient	Not Applicable	Log K_{ow}	6.4	Not Reported	EC, ECB, 2000a
Test material: C9-12 Isoparaffin (CAS# 90622-57-4)					
Octanol-water Partition Coefficient	Not Applicable	Log K_{ow}	4.9-6.9	Not Reported	EC, ECB, 2000b
Bioconcentration Factor (BCF)	Fathead minnow (*Pimephales promelas*)	BCF	3,152-100,000	Calculation	
Test material: Solvent Naphtha (petroleum), Medium Aliphatic (CAS# 64742-88-7)					
Octanol-water Partition Coefficient	Not Applicable	Log K_{ow}	3.3-6	Calculation	EC, ECB, 2000c

Notes:
BCF = Bioconcentration Factor; CAS = Chemistry Abstracts Service; LogK_{ow} = Octanol-water Partition Coefficient.

Due to a lack of bioaccumulation data for ECOSOLV, surrogate data were used to assign a bioaccumulation score. Table 16 presents a summary of octanol-water partition coefficient (Log K_{ow}) and bioconcentration faction (BCF) data for three suitable surrogates. Log K_{ow} values of greater than 5.0 and BCF values of greater than 5,000 indicate that ECOSOLV exhibits very high bioaccumulative potential, in accordance with the GreenScreen guidance for bioaccumulation. Additionally, one of ECOSOLV's surrogates, Solvent naphtha (petroleum), medium aliphatic, is listed as bioaccumulative on a screening list. Therefore, the bioaccumulation score of very high is assigned with high confidence.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): *L*

ECOSOLV is assigned a score of *Low (L)* for reactivity based on professional judgment, using the information below. Low confidence has been assigned to this score.

Authoritative and Screening Lists

- *Authoritative*: Not listed
- *Screening*: Not listed

Labinger and Bercaw (2002)

- ECOSOLV is composed of saturated hydrocarbons, a class of compounds that are relatively inert due to the stability of their chemical bonds. Chemical transformations of saturated hydrocarbons require energy intensive processes, or enzymatic or synthetic catalysis.

Chevron (2014)

- The NFPA classification of ECOSOLV for reactivity is 0.

Summary

While no specific data or information were identified regarding reactivity for ECOSOLV, available information suggests that ECOSOLV does not present a reactivity hazard and has been assigned a score of *Low* (*L*). Low confidence has been assigned to this score due to the lack of supporting data.

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

ECOSOLV is assigned a score of **Moderate (M)** for flammability based on reported flash points, which are greater than 60°C but less than 93°C. Based on GHS criteria, ECOSOLV is classified as a Category 4 flammable liquid. High confidence has been assigned to this score due to the availability of supporting data

Authoritative and Screening Lists

- *Authoritative*: Not listed
- *Screening*: Not listed

ECHA (2015)

- CAS 68551-19-9 is reported to have a flash point of 67°C at 1 atm using ASTM method D 93 .

Chevron (2014)

- ECOSOLV is reported to have a flash point of 61.1°C using a tag closed cup method.
- The NFPA fire hazard classification of ECOSOLV is 1.

Summary

ECOSOLV is assigned a score of **Moderate (M)** for flammability based on reported flash points and GHS classification guidance. High confidence has been assigned to this score due to the availability of supporting data.

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Appendix A

Hazard Benchmark Acronyms

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Hazard Benchmark Acronyms

AA	Acute Aquatic Toxicity
AT	Acute Mammalian Toxicity
B	Bioaccumulation
C	Carcinogenicity
CA	Chronic Aquatic Toxicity
Cr	Corrosion/ Irritation (Skin/ Eye)
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

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Appendix B

PHAROS Results – ECOSOLV and Associated Transformation Products

Toggle navigation Pharos

- Building Products
- Chemicals and Materials
- Certifications
- CompAIR
- Dashboard
- Logout

1. Dashboard
2. Chemicals and Materials
3. [68551-19-9] ALKANES, C12-14-ISO-

[68551-19-9] ALKANES, C12-14-ISO-

- General Information
- Hazards
- Process Chemistry Research
- GreenScreen
- C2C

CAS RN: 68551-19-9

Description: *Not provided*

Website (if applicable): *Not provided*

- View products containing this material

My Project Lists

No project lists available. Lists can be added to existing projects on your account. Visit your dashboard for more information.

Direct Hazards:

None identified

Potential Residual Hazards:

See Process Chemistry Research tab for details on residuals and other substances used in manufacture.

None identified

Process Chemistry Research Status: No life cycle research started

GreenScreen for Safer Chemicals Full Assessment: *None available*

Highest concern GreenScreen score : *Unknown*

Cradle to Cradle Certified™ List Hazards

What are C2C hazards and what do these colors mean?

×

What are C2C hazards and what do these colors mean?

What are the C2C Hazards? The Cradle to Cradle Certified Product Standard establishes a Material Health Assessment Methodology which assigns hazard ratings to 24 individual human and environmental health endpoints. Roll your cursor over the abbreviations (C, M, R+D, etc) in the table to see the full name of each endpoint (Carcinogenicity, Mutagenicity, Reproductive Toxicity, etc). Organohalogen and Toxic Metal are classes of chemicals generally associated with significant human and environmental health issues and are specially treated in the C2C Standard.

The hazard rating is a Green-Yellow-Red-Grey color scheme based upon available toxicity and fate information:

- Green: no hazard identified for the endpoint
- Red: hazard identified for the endpoint
- Yellow: borderline
- Grey: no data available for the endpoint

This tab shows the preliminary hazard ratings based upon hazard lists tracked in the Pharos Chemical & Material Library. During full assessment for certification purposes, Grey hazards must be filled by an accredited assessor and other list-based hazards may be overridden.

Why are these rating colors sometimes different from the GreenScreen or Pharos rating colors? The C2C hazard rating colors are similar to those used in the GreenScreen system and in Pharos, with some distinctions. Pharos has two additional rating colors - orange and purple - not used in the C2C or GreenScreen systems. Pharos orange, red and purple ratings generally encompass the C2C & GreenScreen red ranges. There are some distinctions between the GreenScreen and C2C thresholds that result in different color assignments that are under consideration for harmonization. See the Material Health Evaluation Programs Harmonization Opportunities Report for details. For substances that have been fully assessed under the GreenScreen protocol, there may be different colors due to the application of data from studies that provide information beyond that in the hazard lists.

If interested in assessing the chemicals in a product, please also review the link below describing "How to Use These Scores in a C2C Assessment".

How to Use These Scores in a C2C Assessment

×

How to Use These Scores in a C2C Assessment

The top table displays preliminary hazard ratings for individual endpoints based on the hazard lists a given chemical appears on. During the assessment, an accredited Cradle to Cradle Certified Material Health Assessor may override these list-based hazard ratings based on information from other sources. Additionally, a red hazard rating in any one endpoint does not automatically mean that a substance will be x-assessed and targeted for phase-out, as exposure relevant to the endpoint may be deemed non-plausible for the substance depending on the material and product context in which it is being assessed.

The bottom table (Full Hazard List by Endpoint) includes all warnings associated with the substance from each of the authoritative hazard lists used by C2C, as well as additional lists in the Pharos Chemical and Material

Library. C2C lists are labeled with their C2C hazard rating (Red, Yellow, or Green), while non-C2C lists are labeled as "not rated".

The ratings for the hazard lists used in this tool are based on Table 9 in the Material Assessment Methodology, Cradle to Cradle Certified Version 3.0 with a few minor adjustments/additions to allow for direct mapping from GreenScreen list translator results for a subset of the covered lists. The v3.0 Material Assessment Methdology document can be found on the C2C Resources page at http://www.c2ccertified.org/resources/collection-page/cradle-to-cradle-certified-resources.

Key
R: Red hazard level
Y: Yellow hazard level
G: Green hazard level
?: On a hazard list that has not been rated by C2C
-: Not listed on any C2C or Pharos hazard lists

Acute and Chronic Tox.											Acute Aquatic Tox.				Chronic Aquatic Tox.								
C	**M**	**R+D**	**E**	**O**	**D**	**I**	**O/D/I**	**N**	**IrS+IrE**	**SnS+SnR**	**Fish**	**Inv.**	**Alg.**	**Any**	**Fish**	**Inv.**	**Alg.**	**Any**	**T**	**P**	**B**	**Climate**	**Orga**
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	G	NL

Full Hazard List By Endpoint:

Carcinogenicity	not listed
Mutagenicity	not listed
Reproductive Toxicity (Repro + Dev)	not listed
Endocrine Disruption	not listed
Oral Toxicity	not listed
Dermal Toxicity	not listed
Inhalative Toxicity	not listed
Oral, Dermal, and/or Inhalative Toxicity	not listed
Neurotoxicity	not listed
Skin, Eye, and Respiratory Corrosion/Irritation	not listed
Skin and Respiratory Sensitization	not listed
Acute Aquatic Toxicity (Fish)	not listed
Acute Aquatic Toxicity (Invertibrates)	not listed
Acute Aquatic Toxicity (Algae)	not listed
Acute Aquatic Toxicity (Fish, Invertibrates,	not listed

and/or Algae)	
Chronic Aquatic Toxicity (Fish)	not listed
Chronic Aquatic Toxicity (Invertibrates)	not listed
Chronic Aquatic Toxicity (Algae)	not listed
Chronic Aquatic Toxicity (Fish, Invertibrates, and/or Algae)	not listed
Terrestrial	not listed
Persistence	not listed
Bioaccumulation	not listed
Climatic Relevance	not listed
Organohalogen	not listed - *This chemical is not on the Pharos list of organohalogens, but we may have missed a few. Please double-check the chemical structure to confirm there are no carbon-halogen bonds.*
Toxic Metal	not listed - *This chemical is not on the Pharos list of toxic metals, but we may have missed a few. Please double-check the chemical structure to confirm there are no toxic metals.*
Other (Human Health)	not listed
Multiple Endpoints	not listed

×

Substance Hazard

This color reflects the highest hazard associated directly with this substance by an authoritative hazard list.

The colors represent the relative level of hazard, ranging from **purple** (highest concern) through **red**, **orange**, and **yellow** to **green** (lowest concern).

Grey indicates that the authoritative hazard listing is ambiguous and covers a wide range of possible hazard levels.

Blue indicates that the substance is referenced on a restricted substance list (RSL) rather than an authoritative hazard list.

For a full description of authoritative hazard lists used in Pharos and of the derivation of the hazard level indicators, see the complete Pharos Chemical and Material Library Description.

For the authoritative hazard list that is the source of this hazard color, see the "Hazard" tab on the chemical / material's page.

×

Residual Hazard

This color reflects the highest hazard associated with residual chemicals that our research indicates may be present with the chemical. These residuals consist of all process chemicals in the following categories:

- Monomers

- Catalysts
- Non-reactive Additives
- Pollutants and Contaminants
- Other known residuals

Hazards are drawn from process chemicals far upstream in the manufacturing process as well as the immediate precursors to this chemical.

The colors represent the relative level of hazard, ranging from **purple** (highest concern) through **red**, **orange**, and **yellow** to **green** (lowest concern).

Grey indicates that the authoritative hazard listing is ambiguous and covers a wide range of possible hazard levels.

Blue indicates that the substance is referenced on a restricted substance list (RSL) rather than an authoritative hazard list.

For a full description of authoritative hazard lists used in Pharos and of the derivation of the hazard level indicators, see the complete Pharos Chemical and Material Library Description.

For the source of this hazard, see the "Process Chemistry Research" tab on the chemical's page.

×

Manufacturing Hazard

This color reflects the highest hazard associated with chemicals that our research categorizes as “frequent” or “integral” to the production of a chemical. The manufacturing score is included to surface potential hazards upstream in the manufacturing process that may or may not be present as residuals. Hazards are drawn from process chemicals far upstream in the manufacturing process as well as the immediate precursors to this chemical.

The colors represent the relative level of hazard, ranging from **purple** (highest concern) through **red**, **orange**, and **yellow** to **green** (lowest concern).

Grey indicates that the authoritative hazard listing is ambiguous and covers a wide range of possible hazard levels.

Blue indicates that the substance is referenced on a restricted substance list (RSL) rather than an authoritative hazard list.

For a full description of authoritative hazard lists used in Pharos and of the derivation of the hazard level indicators, see the complete Pharos Chemical and Material Library Description.

For the source of this hazard, see the "Process Chemistry Research" tab on the chemical's page.

×

GreenScreen

The Pharos scoring system is informed by the GreenScreen® for Safer Chemicals, a benchmarking system to rank the safety of chemicals on a 4 point hazard scale and encourage progress toward safer alternatives. Chemicals that have undergone a full GreenScreen assessment by Licensed GreenScreen Profilers are given a Benchmark score, which is the most authoritative. Chemicals that have been assessed using an automated

comparison to hazard lists are given a List Translator score, which is less authoritative. Full GreenScreen assessments trump results from List Translator scoring.

GreenScreen Scores in order from highest concern to lowest concern are:

- Benchmark 1
- LT-1 - List Translator Likely Benchmark 1
- LT-P1 - List Translator Possible Benchmark 1
- LT-UNK - List Translator Benchmark Unknown
- Benchmark U
- Benchmark 2
- Benchmark 3
- Benchmark 4

For more information, see the "GreenScreen" tab on the chemical's page or visit www.greenscreenchemicals.org.

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