

Web-based Applications to Support Access to Chemistry-Related Data

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The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

- The Center for Computational Toxicology and Exposure has delivered many tools to quickly access data for chemicals
 - CompTox Chemicals Dashboard (available since 2016)
(<https://comptox.epa.gov/dashboard>)
 - Cheminformatics modules (6 PoC modules in total)
(<https://www.epa.gov/chemical-research/cheminformatics>)
 - Hazard Profiling
 - Safety Profiling (work in progress)

CompTox Chemicals Dashboard

<https://comptox.epa.gov/dashboard>

CompTox Chemicals Dashboard v2.2.1 Home Search ▾ Lists ▾ About ▾ Tools ▾ Submit Comments

CompTox Chemicals Dashboard

Search 1,200,059 Chemicals

Chemicals

Products/Use Categories

Assay/Gene

vinyl|



Vinyl 1H,1H,3H-perfluoropropyl ether
DTXSID10183954



Vinyl 2,2,5,5-tetramethylhexanoate
DTXSID90233108



Vinyl 2-chlorobenzoate
DTXSID60343086



Vinyl 3-butenate
DTXSID50173132



Vinyl 3-chloro-2,2,3,3-tetrafluoropropanoate
DTXSID50233048



Vinyl 3-Phenylpropanoate
DTXSID40474029



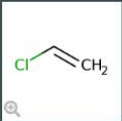
Vinyl 4-(1,1-dimethylethyl)benzoate



1 of ~1.2M Chemical Pages

Accessing various forms of data

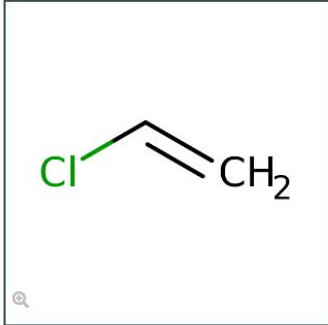
CompTox Chemicals Dashboard v2.2.1 Home Search Lists About Tools Submit Comments Search all data



Vinyl chloride

75-01-4 | DTXSID8021434
Searched by Approved Name.

Chemical Details



Wikipedia

Vinyl chloride is an organochloride with the formula $\text{H}_2\text{C}=\text{CHCl}$. It is also called **vinyl chloride monomer (VCM)** or **chloroethene**. This colorless compound is an important industrial chemical chiefly used to produce the polymer, poly(vinyl chloride) (PVC). Vinyl chloride monomer is among the top twenty largest petrochemicals (petroleum-derived chemicals) in world production. The United States remains the largest vinyl chloride manufacturing region because of its

[Read more](#)

Quality Control Notes

Intrinsic Properties

 Molecular Formula: $\text{C}_2\text{H}_3\text{Cl}$ [MOL FILE](#) [FIND ALL CHEMICALS](#)

 Average Mass: 62.5 g/mol [ISOTOPE MASS DISTRIBUTION](#)

 Monoisotopic Mass: 61.992328 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

- Chemical Details
- Executive Summary
- Physchem Prop.
- Env. Fate/Transport
- Hazard Data
- Safety > GHS Data
- ADME > IVIVE
- Exposure
- Bioactivity
- GenRA
- ACToR
- Literature
- Links
- Comments



Access to the ToxVal Hazard database

Chemical Details ▾

Executive Summary

Physchem Prop.

Env. Fate/Transport

Hazard Data ▾

Hazard

Cancer

Genotoxicity

Skin/Eye

Bioactivity

GenRA

Chemical Details

The image shows the chemical structure of chloroethene (vinyl chloride) in a skeletal format. It consists of a two-carbon chain with a double bond between them. One carbon is bonded to a chlorine atom (Cl) and a hydrogen atom (not explicitly shown). The other carbon is bonded to two hydrogen atoms (CH₂). The Cl atom is colored green, and the CH₂ group is in black. A small magnifying glass icon is located in the bottom-left corner of the structure box.

ClC=CH2

Access to the ToxVal Hazard database

Hazard: Point of Departure

Point of Departure



Search Hazard

☒ human ☐ eco

Point of Departure

Toxicity Value

Lethality Effect Level

Screening Level

Exposure Limit

other

Effect Level

Effect Concentration

Inhibition Concentration

	1	ATSDR MRLs 2020	NOAEL	-	short-term	=	38.3	ppm	short-term	inhalation	developmental	Human (RA)	2006
	1	ATSDR MRLs 2020	NOAEL	-	chronic	=	2.30	ppm	chronic	inhalation	hepatic	Human (RA)	2006
	1	ATSDR MRLs 2020	NOAEL	-	chronic	=	9.00e-2	mg/kg-day	chronic	oral	hepatic	Human (RA)	2006
	1	ATSDR MRLs 2022	NOAEL	-	acute	=	38.3	ppm	acute	inhalation	developmental	Human (RA)	-
	1	ATSDR MRLs 2022	NOAEL	-	short-term	=	2.30	ppm	short-term	inhalation	hepatic	Human (RA)	-
	1	ATSDR MRLs 2022	NOAEL	-	chronic	=	9.00e-2	mg/kg-day	chronic	oral	hepatic	Human (RA)	-
	1	IRIS	NOAEL	-	chronic	=	2.50	mg/m3	chronic	inhalation	Hepatic:Liver cell polymorphism	Human (RA)	-
	1	IRIS	NOAEL	-	chronic	=	9.00e-2	mg/kg-day	chronic	oral	Hepatic:Liver cell polymorphism	Human (RA)	-
	3	DOE Wildlife Benchmark	NOAEL	Test species	chronic	=	0.170	mg/kg-day	chronic	oral	-	Little Brown ...	-
	3	DOE Wildlife Benchmark	NOAEL	Test species	chronic	=	0.170	mg/kg-day	chronic	oral	-	American Sh...	-
	3	DOE Wildlife Benchmark	NOAEL	Test species	chronic	=	0.170	mg/kg-day	chronic	oral	-	White-Footed ...	-
	3	DOE Wildlife Benchmark	NOAEL	Test species	chronic	=	0.170	mg/kg-day	chronic	oral	-	Meadow Vole	-

Rows: 82

Total Rows: 82

Chemical Details

Executive Summary

Physchem Prop.

Env. Fate/Transport

Hazard Data

Hazard

Cancer

Genotoxicity

Skin/Eye

Bioactivity

GenRA

Batch Access to Data

<https://doi.org/10.1021/Facs.jcim.0c01273>

Batch Search

1 Select Input Type(s)

Substance Identifiers

- ☒ Chemical Name
- ☐ CASRN
- ☐ InChIKey
- ☐ DSSTox Substance ID
- ☐ DSSTox Compound ID
- ☐ InChIKey Skeleton
- ☐ MS-Ready Formula(e)
- ☐ Exact Formula(e)
- ☐ Monoisotopic Mass

2 Enter Identifiers to Search

(Please enter one identifier per line and limit the number of identifiers to 10,000 or less)

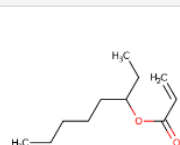
POLYVINYL
POLYPROPYL GLYCOL
ISOBUTYLENE
BUTYL ACRYLATE
ETHYLHEXYL ACRYLATE
PARAFFIN WAX
POLYPROPYLENE
POLYETHYLENE

3 OR

13 Chemicals Found from 14 Input(s)

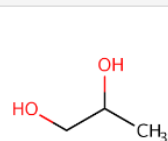
TILE INFO

Showing 13 of 13 chemicals



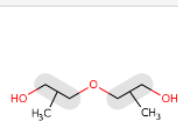
Ethylhexyl acrylate

DTXSID : DTXSID001031472
CASRN : 1322-19-0
TOXCAST :



1,2-Propylene glycol

DTXSID : DTXSID0021206
CASRN : 57-55-6
TOXCAST : 20/909



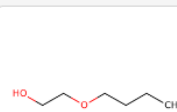
Dipropylene glycol

DTXSID : DTXSID0027856
CASRN : 25265-71-6
TOXCAST : 6/656

1 related chemical structure
with this substance

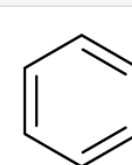
Polypropylene

DTXSID : DTXSID00872805
CASRN : 9003-07-0
TOXCAST :



2-Butoxyethanol

DTXSID : DTXSID1024097
CASRN : 111-76-2
TOXCAST : 7/655



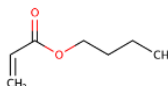
Benzene

DTXSID : DTXSID0039242
CASRN : 71-43-2
TOXCAST : 1/235

0 related chemical structures
with this substance

Paraffin waxes

DTXSID : DTXSID001018729
CASRN : 308059-08-1
TOXCAST :



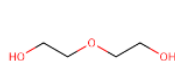
Butyl acrylate

DTXSID : DTXSID0024676
CASRN : 141-32-2
TOXCAST : 16/448

0 related chemical structures
with this substance

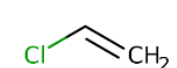
Hydrocarbon waxes

DTXSID : DTXSID0027673
CASRN : 8002-74-2
TOXCAST :



Diethylene glycol

DTXSID : DTXSID0020462
CASRN : 111-46-6
TOXCAST : 7/942



Vinyl chloride

DTXSID : DTXSID0021434
CASRN : 75-01-4
TOXCAST :

1 related chemical structure
with this substance

Polyethylene AS low Mol....

DTXSID : DTXSID0031946
CASRN : 9002-88-4
TOXCAST :

Batch Access to Data

<https://doi.org/10.1021/Facs.jcim.0c01273>

Batch Search

1 Select Input Type(s)

- ☒ Substance Identifiers
- ☒ Chemical Name
 - ☐ CASRN
 - ☐ InChIKey
 - ☐ DSSTox Substance ID
 - ☐ DSSTox Compound ID
 - ☐ InChIKey Skeleton
 - ☐ MS-Ready Formula(e)
 - ☐ Exact Formula(e)
 - ☐ Monoisotopic Mass

2 Enter Identifiers to Search

(Please enter one identifier per line and limit the number of identifiers to 10,000 or less)

POLYVINYL
POLYPROPYL GLYCOL
ISOBUTYLENE
BUTYL ACRYLATE
ETHYLHEXYL ACRYLATE
PARAFFIN WAX
POLYPROPYLENE
POLYETHYLENE

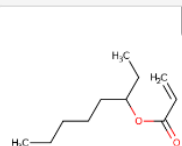
3 or

13 Chemicals Found from 14 Input(s)

TITLE INFO

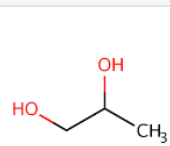
FILTER

Showing 13 of 13 chemicals



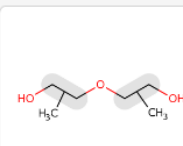
Ethylhexyl acrylate

DTXSID : DTXSID001031472
CASRN : 1322-19-0
TOXCAST :



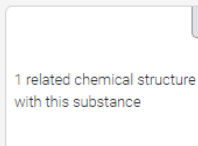
1,2-Propylene glycol

DTXSID : DTXSID0021206
CASRN : 57-55-6
TOXCAST : 20/909



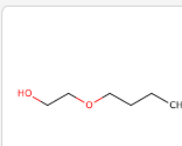
Dipropylene glycol

DTXSID : DTXSID0027856
CASRN : 25265-71-6
TOXCAST : 6/656



Polypropylene

DTXSID : DTXSID00372805
CASRN : 9003-07-0
TOXCAST :



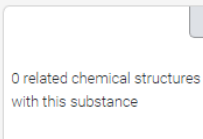
2-Butoxyethanol

DTXSID : DTXSID1024097
CASRN : 111-76-2
TOXCAST : 7/655



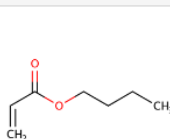
Butyl acrylate

DTXSID : DTXSID0021434
CASRN : 75-01-4
TOXCAST :



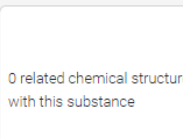
Paraffin waxes

DTXSID : DTXSID001018729
CASRN : 308059-08-1
TOXCAST :



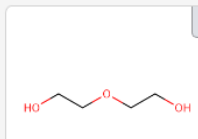
Butyl acrylate

DTXSID : DTXSID0024676
CASRN : 141-32-2
TOXCAST : 16/448



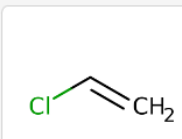
Hydrocarbon waxes

DTXSID : DTXSID0027673
CASRN : 8002-74-2
TOXCAST :



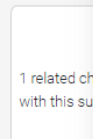
Diethylene glycol

DTXSID : DTXSID0020462
CASRN : 111-45-6
TOXCAST : 7/942



Vinyl chloride

DTXSID : DTXSID0021434
CASRN : 75-01-4
TOXCAST :



Polyethylene

DTXSID : DTXSID0021434
CASRN : 75-01-4
TOXCAST :

4 CHOOSE EXPORT FORMAT

☐ Select All columns available

Chemical Identifiers

- ☒ DTXSID
- ☒ Chemical Name
- ☐ DTXCID
- ☐ CAS-RN
- ☐ InChIKey
- ☐ IUPAC Name

Structures

- ☐ Mol File
- ☐ SMILES
- ☐ InChI String
- ☐ MS-Ready SMILES
- ☐ QSAR-Ready SMILES

Intrinsic and Predicted Properties

- ☐ Molecular Formula
- ☐ Average Mass
- ☐ Monoisotopic Mass
- ☐ TEST Model Predictions
- ☐ OPERA Model Predictions
- ☐ ToxPrint fingerprints (ChemoTyper)
- ☐ ToxPrint single fingerprints

Your file will be exported in Microsoft Excel Format (.xlsx)

Metadata

- ☐ Curation Level Details
- ☐ Safety Data
- ☐ NHANES/Predicted Exposure
- ☐ Data Sources
- ☐ Include ToxVal Data Availability
- ☐ Assay Hit Count
- ☐ Number of PubMed Articles
- ☐ PubChem Data Sources
- ☐ CPDat Product Occurrence Count
- ☐ IRIS
- ☐ PPRTV
- ☐ Wikipedia Article
- ☐ QC Notes
- ☐ Include links to ACToR reports

Enhanced Data Sheets

- ☐ MetFrag Input File (Beta)
- ☐ Abstract Sifter Input File
- ☐ Synonyms and Identifiers
- ☐ Related Substance relationships
- ☐ Associated ToxCast Assays
- ☐ ToxValDB Details
- ☐ Physicochemical Property Values

Data visualizations are increasingly necessary

- >1800 rows of hazard data for a dozen chemicals
- Is there an easier way to view complex hazard data?

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	
714	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Carcinoge	LOAEC	LOAEC	-		Point of D	LOAEC	=	127.812	50	ppm	ppm	chronic	chronic	carcinoger	-
715	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Carcinoge	LOAEC	LOAEC	-		Point of D	LOAEC	=	12781.2	5000	ppm	ppm	chronic	chronic	carcinoger	-
716	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Carcinoge	LOAEL	LOAEL	-		Point of D	LOAEL	=	1.7	1.7	mg/kg-da	mg/kg bw	chronic	chronic	carcinoger	-
717	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Carcinoge	NOAEL	NOAEL	-		Point of D	NOAEL	=	0.13	0.13	mg/kg-da	mg/kg bw	chronic	chronic	carcinoger	-
718	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Developm	LOAEC	LOAEC	-		Point of D	LOAEC	=	500	500	ppm	ppm	developm	developm	developm	-
719	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Developm	NOAEC	NOAEC	-		Point of D	NOAEC	=	10	10	ppm	ppm	developm	developm	developm	-
720	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Developm	NOAEC	NOAEC	-		Point of D	NOAEC	=	50	50	ppm	ppm	developm	developm	developm	-
721	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Developm	NOAEC	NOAEC	-		Point of D	NOAEC	=	2500	2500	ppm	ppm	developm	developm	developm	-
722	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	LOAEC	LOAEC	-		Point of D	LOAEC	=	127.812	50	ppm	ppm	chronic	chronic	chronic to	-
723	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	LOAEC	LOAEC	-		Point of D	LOAEC	=	12781.2	5000	ppm	ppm	chronic	chronic	chronic to	-
724	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	LOAEC	LOAEC	-		Point of D	LOAEC	=	51125	20000	ppm	ppm	subchroni	subchroni	sub-chron	-
725	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	LOAEC	LOAEC	-		Point of D	LOAEC	=	127812	50000	ppm	ppm	short-term	short-term	short-term	-
726	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	LOEC	LOEC	-		Point of D	LOEC	=	260	260	mg/m3	mg/m3 air	chronic	chronic	repeated c	-
727	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	NOAEC	NOAEC	-		Point of D	NOAEC	=	127.812	50	ppm	ppm	subchroni	subchroni	sub-chron	-
728	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	NOAEC	NOAEC	-		Point of D	NOAEC	=	255.625	100	ppm	ppm	subchroni	subchroni	sub-chron	-
729	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	NOAEC	NOAEC	-		Point of D	NOAEC	=	511.25	200	ppm	ppm	subchroni	subchroni	sub-chron	-
730	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	NOEC	NOEC	-		Point of D	NOEC	=	130	130	mg/m3	mg/m3 air	repeat do	repeat do	repeated c	-
731	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	LOAEL	LOAEL	-		Point of D	LOAEL	=	1.7	1.7	mg/kg-da	mg/kg bw	chronic	chronic	chronic to	-
732	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	NOAEL	NOAEL	-		Point of D	NOAEL	=	0.13	0.13	mg/kg-da	mg/kg bw	chronic	chronic	chronic to	-
733	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECHA IUCI Repeated	NOAEL	NOAEL	-		Point of D	NOAEL	=	30	30	mg/kg-da	mg/kg bw	subchroni	subchroni	sub-chron	-
734	Vinyl chlor	DTXSID80	75-01-4	Vinyl chlor	ECOTOX	EPA ORD	EC50	EC50	active ingr	Effect Con	EC	=	1170	1.17	mg/m3	mg/L	other	population	Population ch	-
Cover Sheet				Main Data				Associated ToxCast Assays				Toxval Details								

- Proof-of-concept tools are to try out new approaches to visualizing and integrating data

Cheminformatics Modules

version: DEV, build: 2023-03-09 06:08:29 UTC

HAZARD

ALERTS

PREDICT 1.0

PREDICT 2.0

SEARCH

STANDARDIZE

TOXPRINTS

↑

Full

🔍

+

✖

🗑

Chemicals: 388

Toxicity: VH - Very High H - High M - Medium L - Low I - Inconclusive N/A - Not Applicable Authority: **Authoritative** [ⓘ] Screening [ⓘ] QSAR Model [ⓘ]

☐ Skipped (0)

☐ Unlikely (0)

☐ Filters (0)

☒ Sorting (0)

☐ Structure

CAS Name

Human Health Effects

Ecotoxicity

Fate

CAS Name	Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Exposure
	Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure								
106-93-4 ^{AIGBT} 1,2-Dibromoethane	H	H	H	VH	VH	H	M	H		H	M	M	I	H	H	H	H	M	L	H
10061-02-6 ^{GBT} trans-1,3-Dichlor...	M				VH	L		L								H		M	L	M
75-44-5 ^{IGBT} Phosgene	VH	VH	I	I	L	L	I	L			H	H	I	VH	VH	I	I	M	L	VH
75-02-5 ^{GBT} Vinyl fluoride	H	L	I	VH	VH	L	I	H			M		I	I	I	L	I	M	L	H
127-91-3 ^{GBTMM} beta-Pinene	L	H	L	I	L	L	I	L	I		I	M	H	H	H	VH	VH	M	L	M
7803-62-5 ^{GBT} Silane	I	M	I	I	I		I	I			M	M	I	H	H	L	I		L	
106-43-4 ^{GBTM} 4-Chlorotoluene	M	M	L	I	L		H	H	I	I	L	I	H	L	H	H	M	M	L	H

How easy is it to source screening data?

ORIGINAL DATA

POLYPROPYLENE
POLYETHYLENE
Residue lube oil
VINYL CHLORIDE
DIPROPYLENE GLYCOL
PROPYLENE GLYCOL
DIETHYLENE GLYCOL
COMBUSTIBLE LIQ., NOS (ETHYLENE GLYCOL MONOBUTYL ETHER)
SEMOLINA
COMBUSTIBLE LIQ., NOS (ETHYLHEXYL ACRYLATE)
POLYVINYL
PETROLEUM LUBEOIL
POLYPROPYL GLYCOL
ISOBUTYLENE
BUTYL ACRYLATES, STABILIZED
PETRO OIL, NEC
ADDITIVES, FUEL
BALLS, CTN, M EDCL
SHEET STEEL
VEGETABLE, FROZEN
BENZENE
PARAFFIN WAX
FLAKES, POWDER
HYDRAULIC CEMENT
AUTOS PASSENGER
MALT LIQUORS

How easy is it to source screening data?

ORIGINAL DATA

POLYPROPYLENE
POLYETHYLENE
Residue lube oil
VINYL CHLORIDE
DIPROPYLENE GLYCOL
PROPYLENE GLYCOL
DIETHYLENE GLYCOL
COMBUSTIBLE LIQ., NOS (ETHYLENE GLYCOL MONOBUTYL ETHER)
SEMOLINA
COMBUSTIBLE LIQ., NOS (ETHYLHEXYL ACRYLATE)
POLYVINYL
PETROLEUM LUBEOIL
POLYPROPYL GLYCOL
ISOBUTYLENE
BUTYL ACRYLATES, STABILIZED
PETRO OIL, NEC
ADDITIVES, FUEL
BALLS, CTN, M EDCL
SHEET STEEL
VEGETABLE, FROZEN
BENZENE
PARAFFIN WAX
FLAKES, POWDER
HYDRAULIC CEMENT
AUTOS PASSENGER
MALT LIQUORS

FILTERED DOWN TO

VINYL CHLORIDE
DIPROPYLENE GLYCOL
PROPYLENE GLYCOL
DIETHYLENE GLYCOL
ETHYLENE GLYCOL MONOBUTYL
ETHER
POLYVINYL
POLYPROPYL GLYCOL
ISOBUTYLENE
BUTYL ACRYLATE
ETHYLHEXYL ACRYLATE
PARAFFIN WAX
POLYPROPYLENE
POLYETHYLENE

Hazard Comparison Profiling

Search by identifiers

Retrieve Comptox List

Search by structure

Search result

BENZENE

VINYL CHLORIDE

DIPROPYLENE GLYCOL

PROPYLENE GLYCOL

DIETHYLENE GLYCOL

ETHYLENE GLYCOL MONOBUTYL ETHER

POLYVINYL

POLYPROPYL GLYCOL

ISOBUTYLENE

BUTYL ACRYLATE

SEARCH

Hazard Comparison Profiling

Search by identifiers

Retrieve Comptox List

Search by structure

Search result

BENZENE

VINYL CHLORIDE

DIPROPYLENE GLYCOL

PROPYLENE GLYCOL

DIETHYLENE GLYCOL

ETHYLENE GLYCOL MONOBUTYLENE GLYCOL

POLYVINYL

POLYPROPYLENE GLYCOL

ISOBUTYLENE

BUTYL ACRYLATE

Search by identifiers

Retrieve Comptox List

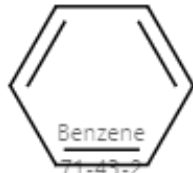
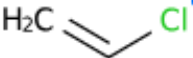
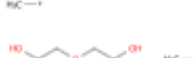
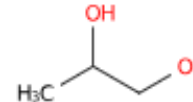
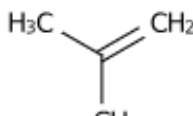
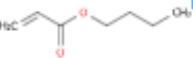
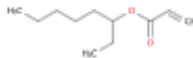
Search by structure

Search result

Chemical(s) found by 14 identifier(s)

12 / 15



 Benzene 71-43-2 BENZENE	 Vinyl chloride 75-01-4 VINYL CHLORIDE	 Dipropylene glycol 25265-71-8 DIPROPYLENE GLYCOL	 1,2-Propylene glycol 57-55-6 PROPYLENE GLYCOL	 Diethylene glycol 111-46-6 DIETHYLENE GLYCOL	 2-Butoxyethanol 111-76-2 ETHYLENE GLYCOL M...
 Isobutylene 115-11-7 ISOBUTYLENE	 Butyl acrylate 141-32-2 BUTYL ACRYLATE	 Ethylhexyl acrylate 1322-13-0 ETHYLHEXYL ACRYLATE	 Hydrocarbon waxes 8002-74-2 PARAFFIN WAX	 Polypropylene 9003-07-0 POLYPROPYLENE	 Polyethylene AS low ... 9002-88-4 POLYETHYLENE

☒ Found (12) ☐ Unresolved (2) ☐ Duplicate (1)

Hazard Comparison Profiling

Chemicals: 12

Toxicity: VH - Very High H - High M - Medium L - Low I - Inconclusive N/A - Not Applicable Authority: Authoritative Screening QSAR Model

CAS Name	Human Health Effects															Ecotoxicity		Fate		
	Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity/Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Exposure
	Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure								
☒ CAS Name 71-43-2 Benzene AIGBT	M	L	VH	VH	VH	H	H	H	H		H	H	I	H	H	H	M	M	H	H
☒ CAS Name 75-01-4 Vinyl chloride AIGBT	M	L	I	VH	VH	L	M	M	H	H	H		M	H	I	M	VH	M	L	VH
☒ CAS Name 25265-71-8 Dipropylene glycol GBT	L	I	L		L		L	L			L			M	H	L			L	
☒ CAS Name 57-55-6 1,2-Propylene glycol AIGBT	L	I	L	L	VH	H	L	H	H	H	H		L	L	L	L	L	L	L	VH
☒ CAS Name 111-46-6 Diethylene glycol GBTM	M	I	L	I	L	H	M	L		I	H	I	L	L	L	L	L	L	L	VH
☒ CAS Name 111-76-2 2-Butoxyethanol AIGBT	M	M	M	L	VH	H	M	L		H	H	H	L	H	H	L	L	L	L	VH
☒ CAS Name 115-11-7 Isobutene GBTM	I	L	I	I	L	L	I	H	L	I	H	I	I	I	I	L		M	L	VH
☒ CAS Name 141-32-2 Butyl acrylate GBTM	M	H	M	I	L	L	M	L			M	M	H	H	H	H	H	L	L	H
☒ CAS Name 1322-13-0 Ethylhexyl acrylate GBT	L				L	L		L								VH			I	
☒ CAS Name 8002-74-2 Hydrocarbon waxes GBT	L	I	L	I	L		L	I	I		H	M	I	L	M	L	I		L	
☒ CAS Name 9003-07-0 Polypropylene GBT				I												L			L	
☒ CAS Name 9002-88-4 Polyethylene AS I... GBT		M		I												L			L	

Hazard Profile

Underlying data available

- Underlying toxicity data are from ToxVal and integrated GHS data
- Build a hazard profile on 500 chemicals in <60s
- Report data in Excel format for easy distribution...

Carcinogenicity for Vinyl chloride (75-01-4)

Toxicity: **VH** - Very High **H** - High **M** - Medium **L** - Low **I** - Inconclusive N/A - Not Applicable Authority: **Authoritative** [ⓘ] Screening [ⓘ] QSAR Model [ⓘ]

Source	Score	Route	Test Organism	Test Type	Category	Hazard Code	Hazard Statement	Rationale	Note
ECHA CLP	VH				Carc. 1A	H350	May cause cancer	Score of VH was assigned based on a hazard code of H350	
EPA mid-Atlantic Region Human Health Risk-Based Concentrations	VH				Carcinogen			Score of VH was assigned on having a value for the cancer slope factor (SFO)	Source: I = IRIS
Germany	VH				Category 1			Score of VH was assigned based on a carcinogenicity category of Category 1	
ToxVal (Cal OEHA)	VH	inhalation	-	cancer unit risk				A cancer unit risk indicates carcinogenicity in humans.	
ToxVal (Cal OEHA)	VH	inhalation	-	cancer slope factor				A cancer slope factor is assessed if Hazard Identification provides evidence of human carcinogenicity.	

EPA
United States
Environmental Protection
Agency

AutoSave Off

Hazard Profiling of East Palestine chemicals.xlsx

No Label • Last Modified: 3m ago

Williams, Antony (he/him/his)

FileHomeInsertDrawPage LayoutFormulasDataReviewViewDeveloperHelp

Clipboard

Font

Alignment

Number

Styles

Cells

Editing

Sensitivity

A1

The Hazard Comparison Dashboard is a prototype tool and a compilation of information sourced from many sites, databases and sources including U.S. Federal

The Hazard Comparison Dashboard is a prototype tool and a compilation of information sourced from many sites, databases and sources including U.S. Federal and state sources and international bodies that saves the user time. The data are not reviewed by USEPA – the user must apply judgment in use of the information. The results do not indicate EPA's position on the use or regulation of these chemicals.																	
			VH - Very High		H - High		M - Medium		L - Low		I - Inconclusive		No Data		Authoritative		
			Human Health Effects														
			Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation
			Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure			
DTXSID	CAS	Name															
DTXSID3039242	71-43-2	Benzene	M	L	VH	VH	VH	H	H	H	H		H	H	I	H	H
DTXSID8021434	75-01-4	Vinyl chloride	M	L	I	VH	VH	L	M	M	H	H	H		M	H	I
DTXSID0027856	25265-71-8	Dipropylene glycol	L	I	L		L		L	L			L			M	H
DTXSID0021206	57-55-6	1,2-Propylene glycol	L	I	L	L	VH	H	L	H	H	H	H		L	L	L
DTXSID8020462	111-46-6	Diethylene glycol	M	I	L	I	L	H	M	L		I	H	I	L	L	L
DTXSID1024097	111-76-2	2-Butoxyethanol	M	M	M	L	VH	H	M	L		H	H	H	L	H	H
DTXSID9020748	115-11-7	Isobutene	I	L	I	I	L	L	I	H	L	I	H	I	I	I	I
DTXSID6024676	141-32-2	Butyl acrylate	M	H	M	I	L	L	M	L			M	M	H	H	H
DTXSID001031472	1322-13-0	Ethylhexyl acrylate	L				L	L		L							

Hazard Profiles

Hazard Records

All Underlying Data Reported Out

- Harvesting screening data easily, assembled from multiple resources is a key advantage
- Identification of authoritative, screening and predicted data

	A	B	C	D	E	F	G	H	
1	Hazard Name	CAS	Name	Source	Original Source	List Type	Score	Rationale	Route
234	Carcinogenicity	75-01-4	Vinyl chloride	ToxVal	CalEPA	Authoritative	VH	Score of VH was assigned based on a cancer call of "Likely H	
235	Carcinogenicity	75-01-4	Vinyl chloride	Canada		Screening	VH	Score of VH was assigned based on a hazard code of H350	
236	Carcinogenicity	75-01-4	Vinyl chloride	Health Canada Pri		Screening	VH	Score of VH was assigned on based on a category of Carcino	
237	Carcinogenicity	75-01-4	Vinyl chloride	Japan		Screening	VH	Score of VH was assigned based on a hazard code of H350	
238	Carcinogenicity	75-01-4	Vinyl chloride	Malaysia		Screening	VH	Score of VH was assigned based on a hazard code of H350	
239	Carcinogenicity	75-01-4	Vinyl chloride	New Zealand		Screening	VH	Score was assigned based on a category of Category 6.7A (C	
240	Carcinogenicity	75-01-4	Vinyl chloride	TSCA work plan		Screening	VH	Score of VH was assigned based on a category of Known hur	
241	Carcinogenicity	75-01-4	Vinyl chloride	ToxVal	Health Canada	Screening	VH	A cancer slope factor is assessed if Hazard Identification pro oral	
242	Carcinogenicity	75-01-4	Vinyl chloride	ToxVal	Health Canada	Screening	VH	A cancer slope factor is assessed if Hazard Identification pro oral	
243	Carcinogenicity	75-01-4	Vinyl chloride	ToxVal	Pennsylvania DEP ToxValues	Screening	VH	A cancer slope factor is assessed if Hazard Identification pro -	
244	Carcinogenicity	75-01-4	Vinyl chloride	ToxVal	Pennsylvania DEP ToxValues	Screening	VH	A cancer unit risk indicates carcinogenicity in humans.	-
245	Carcinogenicity	75-01-4	Vinyl chloride	ToxVal	Wignall	Screening	VH	A cancer slope factor is assessed if Hazard Identification pro oral	
246	Carcinogenicity	75-01-4	Vinyl chloride	ToxVal	Health Canada	Screening	VH	Score of VH was assigned based on a cancer call of "Group I:	
247	Carcinogenicity	75-01-4	Vinyl chloride	ToxVal	Health Canada	Screening	VH	Score of VH was assigned based on a cancer call of "Group I:	
248	Carcinogenicity	75-01-4	Vinyl chloride	UMD		Screening	VH	Score of VH was assigned based on a category of Carcinogen	
249	Genotoxicity Mutagenicity	75-01-4	Vinyl chloride	EPA mid-Atlantic R		Authoritative	VH	Score of VH was assigned based on a category of M (mutage	
250	Genotoxicity Mutagenicity	75-01-4	Vinyl chloride	New Zealand		Screening	VH	Score was assigned based on a category of Category 6.6A (C	
251	Genotoxicity Mutagenicity	75-01-4	Vinyl chloride	ToxVal		Screening	VH	Score of VH was assigned based on a genetox call of "gentox	
252	Genotoxicity Mutagenicity	75-01-4	Vinyl chloride	Canada		Screening	H	Score of H was assigned based on a hazard code of H341	
253	Genotoxicity Mutagenicity	75-01-4	Vinyl chloride	Japan		Screening	H	Score of H was assigned based on a hazard code of H341	

Work in Progress: Safety Profiling

version: , build:																																
HAZARD SAFETY ALERTS PREDICT 1.0 PREDICT 2.0 SEARCH STANDARDIZE TOXPRINTS																																
↑ Search chemical by Name, CASRN or DTXSID 🔍 Show Structure Full 📄 📄 📄 📄 🗑️																																
Chemical	Safety	Properties	Signal	Explosive	Flammable	Oxidizers	Compressed Gas	Corrosive	Acute Toxicity	Irritant	Health Hazard	Env. Hazard	NFPA 704	Fire Fighting	Accidental Release Measures	Handling and Storage	Stability and Reactivity	Transport Information	Regulatory Information	Other Safety Information	RQ Category	RQ in pounds (kilograms)										
AIGBT													140 30 30																			
71-43-2 Benzene			Danger										140 30 30								A	10 (4.54)										
AIGBT													342 42 42																			
75-01-4 Vinyl chloride			Danger										342 42 42																			
25265-71-8 GBT Dipropylene glycol																																
57-55-6 AIGBT 1,2-Propylene glycol													010 00 00																			
111-46-6 GBTM Diethylene glycol													110 10 10																			
111-76-2 AIGBT 2-Butoxyethanol													320 30 30																			
115-11-7 GBTM Isobutene													241 20 20																			
141-32-2 GBTM Butyl acrylate													322 30 30																			
1322-13-0 Ethylhexyl acrylate																																
1322-13-0 GBT Ethylhexyl acrylate																																
The Cheminformatics Modules is a set of prototype modules which are using a compilation of information sourced from many sites, databases and sources including U.S. Federal and state sources and international bodies that saves the user time by providing information in one location. The data are not reviewed by USEPA – the user must apply judgment in use of the information. The results do not indicate EPA's position on the use or regulation of these chemicals.																																

- Safety data includes
 - GHS data

Pictogram(s)	 
Signal	Danger
GHS Hazard Statements	H220: Extremely flammable gas [Danger Flammable gases] H350: May cause cancer [Danger Carcinogenicity]
Precautionary Statement Codes	P203, P210, P222, P230, P280, P318, P377, P381, P403, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
► EU REGULATION (EC) No 1272/2008	
Pictogram(s)	  
Signal	Danger
GHS Hazard Statements	H220 (100%): Extremely flammable gas [Danger Flammable gases] H280 (69.37%): Contains gas under pressure; may explode if heated [Warning Gases under pressure] H341 (11.95%): Suspected of causing genetic defects [Warning Germ cell mutagenicity] H350 (100%): May cause cancer [Danger Carcinogenicity] H412 (11.95%): Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

- Safety data includes
 - GHS data
 - Firefighting procedures

Excerpt from ERG Guide 116(P) [Gases - Flammable (Unstable); polymerization hazard]:

DO NOT EXTINGUISH A LEAKING GAS FIRE UNLESS LEAK CAN BE STOPPED.

SMALL FIRE: Dry chemical or CO2.

LARGE FIRE: [Water](#) spray or fog. If it can be done safely, move undamaged containers away from the area around the fire.

FIRE INVOLVING TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Cool containers with flooding quantities of [water](#) until well after fire is out. Do not direct [water](#) at source of leak or safety devices; icing may occur. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. For massive fire, use unmanned master stream devices or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2020)

► [CAMEO Chemicals](#)

Shut off supply; if not possible and no risk to surroundings, let the fire burn itself out. In other cases extinguish with powder, [carbon dioxide](#), [water](#) spray. In case of fire: keep cylinder cool by spraying with [water](#). Combat fire from a sheltered position.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

[Fire Fighting Procedures](#) ⓘ

[Firefighting Hazards](#) ⓘ

- Safety data includes
 - GHS data
 - Firefighting procedures
 - Accidental release measures

[Isolation and Evacuation ⓘ](#) ▼

[Spillage Disposal ⓘ](#) ^

Evacuate danger area! Consult an expert! Personal protection: complete protective clothing including self-contained breathing apparatus. Ventilation. Remove all ignition sources. Remove vapour cloud with fine [water](#) spray. NEVER direct [water](#) jet on liquid.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

[Cleanup Methods ⓘ](#) ▼

[Disposal Methods ⓘ](#) ▼

[Preventive Measures ⓘ](#) ▼

- Safety data includes
 - GHS data
 - Firefighting procedures
 - Accidental release measures
 - Transport information

DOT Emergency Guidelines ⓘ	▼
DOT ID and Guide ⓘ	▼
Shipping Name/ Number DOT/UN/NA/IMO ⓘ	▼
Standard Transportation Number ⓘ	▼
Shipment Methods and Regulations ⓘ	▼
DOT Label ⓘ	▼
EC Classification ⓘ	
Symbol: F+, T; R: 45-12; S: 53-45; Note: D	
▶ ILO-WHO International Chemical Safety Cards (ICSCs)	
UN Classification ⓘ	

- Safety data includes
 - GHS data
 - Firefighting procedures
 - Accidental release measures
 - Transport information
 - Toxic combustion products

[Toxic Combustion Products](#) ⓘ

Combustion may produce irritants and toxic gases, including [hydrogen chloride](#), [carbon monoxide](#), [Vinyl chloride](#), inhibited/

Poisonous gases are produced in fire, including [phosgene](#), [hydrogen chloride](#), and [carbon monoxide](#).

The substance decomposes on burning to produce toxic and corrosive fumes ([hydrogen chloride](#), [phosgene](#)).

► [Hazardous Substances Data Bank \(HSDB\)](#)

[History and Incidents](#) ⓘ

[Special Reports](#) ⓘ

Safety Profiling (work-in-progress)

- Safety data includes
 - GHS data
 - Firefighting procedures
 - Accidental release measures
 - Transport information
 - Toxic combustion products
 - History and Incidents

History and Incidents ⓘ

In 2012 in New Jersey, a train derailment resulted in the puncture of a tanker car carrying liquid [vinyl chloride](#) under pressure, and a resulting airborne [vinyl chloride](#) plume drifted onto the grounds of a nearby refinery. This report details the investigation of exposures and symptoms among refinery workers. The investigation team met with refinery workers to discuss their experience after the derailment and provided workers a self-administered survey to document symptoms and worker responses during the incident. Associations among categorical variables and experiencing symptoms were evaluated using Fisher's exact test. Twenty-six of 155 (17 percent) workers present at the refinery or driving on the access road the date the spill occurred completed the survey. Any self-reported symptom following exposure from the [vinyl chloride](#) release /was analyzed/. Fifteen workers (58 percent) reported ≥ 1 symptom, most commonly headache (12, 46 percent). Three (12 percent) reported using respiratory protection. No differences in reporting symptoms were observed by location during the incident or by the building in which workers sheltered. Workers who moved from one shelter to another during the incident (ie, broke shelter) were more likely to report symptoms (Fisher's exact test, $p=0.03$); however, there are only limited data regarding [vinyl chloride](#) concentrations in shelters versus outside. Breaking shelter might result in greater exposures, and managers and health and safety officers of vulnerable facilities with limited physical access should consider developing robust shelter-in-place plans and alternate emergency egress plans. Workers should consider using respiratory protection if exiting a shelter is necessary during a chemical incident.

On November 30, 2012, at approximately 7:00 am, a freight train derailed near a small town in New Jersey. Four tank cars, including a breached tank car carrying [vinyl chloride](#), leaked in a tidal creek. [Vinyl chloride](#) is a colorless gas with a mild, sweet odor, used in plastics manufacture.

Historical Data can be very useful

History and Incidents ⓘ

In 2012 in New Jersey, a train derailment resulted in the puncture of a tanker car carrying liquid [vinyl chloride](#) under pressure, and a resulting airborne [vinyl chloride](#) plume drifted onto the grounds of a nearby refinery. This report details the investigation of exposures and symptoms among refinery workers. The investigation team met with refinery workers to discuss their experience after the derailment and provided workers a self-administered survey to document symptoms and worker responses during the incident. Associations among categorical variables and experiencing symptoms were evaluated using Fisher's exact test. Twenty-six of 155 (17 percent) workers present at the refinery or driving on the access road the date the spill occurred completed the survey. Any self-reported symptom following exposure from the [vinyl chloride](#) release /was analyzed/. Fifteen workers (58 percent) reported ≥ 1 symptom, most commonly headache (12, 46 percent). Three (12 percent) reported using respiratory protection. No differences in reporting symptoms were observed by location during the incident or by the building in which workers sheltered. Workers who moved from one shelter to another during the incident (ie, broke shelter) were more likely to report symptoms (Fisher's exact test, $p=0.03$); however, there are only limited data regarding [vinyl chloride](#) concentrations in shelters versus outside. Breaking shelter might result in greater exposures, and managers and health and safety officers of vulnerable facilities with limited physical access should consider developing robust shelter-in-place plans and alternate emergency egress plans. Workers should consider using respiratory protection if exiting a shelter is necessary during a chemical incident.

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- RapidTox is being developed for multiple workflows
- Internal only *at present* – production system learning from our PoC developments and with a focus on curated data



Emergency Response



Human Health Assessment (V.1.0.0)



Mixture Assessment

- US-EPA-CCTE has delivered tools to access data which can support rapid chemical assessment
 - CompTox Chemicals Dashboard
 - Cheminformatics Modules
- Internal Tools which will go public in the future
 - Safety Profiler
 - RapidTox
- Data caveats: always expanding and always under curation