

US-EPA Web-based Delivery of Chemical Hazard and Safety 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 EPA Center for Computational Toxicology and Exposure has delivered many tools to quickly access data for chemicals
 - Cheminformatics modules (<https://hcd.rtpnc.epa.gov/#/>)
 - Hazard Profiling
 - Safety Profiling
 - AMOS – Analytical methods and Open Spectra

Emergency Response data harvesting

- Example application: How fast could we harvest data during an emergency response event?
- Access to toxicity data, safety data, chemical fact sheets, analytical methods etc.
- Consider the East Palestine Train Derailment



How easy is it to source screening data?

ORIGINAL REPORTED 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

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PARAFFIN WAX
FLAKES, POWDER
HYDRAULIC CEMENT
AUTOS PASSENGER
MALT LIQUORS

FILTERED TO CHEMICALS

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

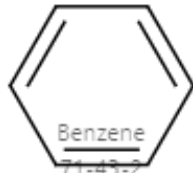
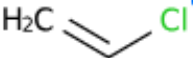
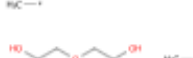
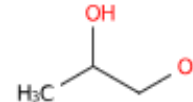
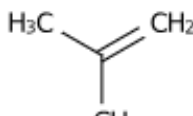
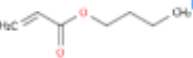
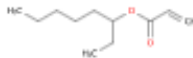
Hazard Comparison Profiling

Search by identifiers Retrieve Comptox List Search by structure Search result

BENZENE
VINYL CHLORIDE
DIPROPYLENE GLYCOL
PROPYLENE GLYCOL
DIETHYLENE GLYCOL
ETHYLENE GLYCOL MONOBUTYLENE
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

Skipped (0)

Unlikely (0)

Filters (0)

Sorting (0)

Structure

CAS

Name

Acute Mammalian Toxicity

Oral

Inhalation

Dermal

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

71-43-2

AIGBT

Benzene

M

L

VH

VH

VH

H

H

H

H

H

H

I

H

H

H

M

M

H

H

75-01-4

AIGBT

Vinyl chloride

M

L

I

VH

VH

L

M

M

H

H

H

M

H

I

M

VH

M

L

VH

25265-71-8

GBT

Dipropylene glycol

L

I

L

L

L

L

L

M

H

L

L

57-55-6

AIGBT

1,2-Propylene glycol

L

I

L

L

VH

H

L

H

H

H

L

L

L

L

L

L

L

VH

111-46-6

GBTM

Diethylene glycol

M

I

L

I

L

H

M

L

I

H

I

L

L

L

L

L

L

VH

111-76-2

AIGBT

2-Butoxyethanol

M

M

M

L

VH

H

M

L

H

H

H

L

H

H

L

L

L

VH

115-11-7

GBTM

Isobutene

I

L

I

I

L

L

I

H

L

I

H

I

I

I

I

L

M

L

VH

141-32-2

GBTM

Butyl acrylate

M

H

M

I

L

L

M

L

M

M

H

H

H

H

H

L

L

H

1322-13-0

Ethylhexyl acrylate

L

L

L

L

VH

I

8002-74-2

GBT

Hydrocarbon waxes

L

I

L

I

L

L

I

I

H

M

I

L

M

L

I

L

9003-07-0

GBT

Polypropylene

I

L

L

9002-88-4

GBT

Polyethylene AS I...

M

I

L

L

Easy Export of all data to Excel

AutoSave Off Hazard Profiling of East Palestine chemicals.xlsx No Label • Last Modified: 3m ago Williams, Antony (he/him/his)

File Home Insert Draw Page Layout Formulas Data Review View Developer Help

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.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	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.																	
2				VH - Very High	H - High	M - Medium	L - Low	I - Inconclusive	No Data	Authoritative								
3				Human Health Effects														
4				Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation
5	DTXSID	CAS	Name	Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure			
6	DTXSID3039242	71-43-2	Benzene	M	L	VH	VH	VH	H	H	H	H		H	H	I	H	H
7	DTXSID8021434	75-01-4	Vinyl chloride	M	L	I	VH	VH	L	M	M	H	H	H		M	H	I
8	DTXSID0027856	25265-71-8	Dipropylene glycol	L	I	L		L		L	L			L			M	H
9	DTXSID0021206	57-55-6	1,2-Propylene glycol	L	I	L	L	VH	H	L	H	H	H	H		L	L	L
10	DTXSID8020462	111-46-6	Diethylene glycol	M	I	L	I	L	H	M	L		I	H	I	L	L	L
11	DTXSID1024097	111-76-2	2-Butoxyethanol	M	M	M	L	VH	H	M	L		H	H	H	L	H	H
12	DTXSID9020748	115-11-7	Isobutene	I	L	I	I	L	L	I	H	L	I	H	I	I	I	I
13	DTXSID6024676	141-32-2	Butyl acrylate	M	H	M	I	L	L	M	L			M	M	H	H	H
14	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	

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																						
71-43-2 Benzene			Danger										  								A	10 (4.54)
AIGBT																						
75-01-4 Vinyl chloride			Danger										  									
GBT																						
25265-71-8 Dipropylene glycol																						
AIGBT																						
57-55-6 1,2-Propylene glycol													  									
GBTM																						
111-46-6 Diethylene glycol			Danger										  									
AIGBT																						
111-76-2 2-Butoxyethanol			Danger										  									
GBTM																						
115-11-7 Isobutene			Danger										  									
GBTM																						
141-32-2 Butyl acrylate			Danger										  									
GBTM																						
1322-13-0 Ethylhexyl acrylate																						
GBT																						

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.

10

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](#), derailed in a tidal creek. [Vinyl chloride](#) is a colorless gas with a mild, sweet odor, and is 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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- US-EPA-CCTE has delivered tools to access data which can support rapid chemical assessment and emergency response
 - Cheminformatics Modules
 - Hazard Module – hazard profiling of chemicals
 - Safety Module – safety data for chemicals
 - AMOS – Analytical Methods and Open Spectra
- Data caveats: always expanding and always under curation

- Cheminformatics Modules (CIM): <https://hcd.rtpnc.epa.gov/>
- Online Manuals:
 - CIM <https://www.epa.gov/comptox-tools/cheminformatics-modules-manual>
 - AMOS <https://www.epa.gov/comptox-tools/analytical-methods-and-open-spectral-amos-database-user-guide>
- Contact Antony Williams with any questions and/or requests for training: williams.antony@epa.gov