

The CompTox Chemistry Dashboard v2.6 – Delivering Improved Access to Data and Real Time Predictions

Antony Williams

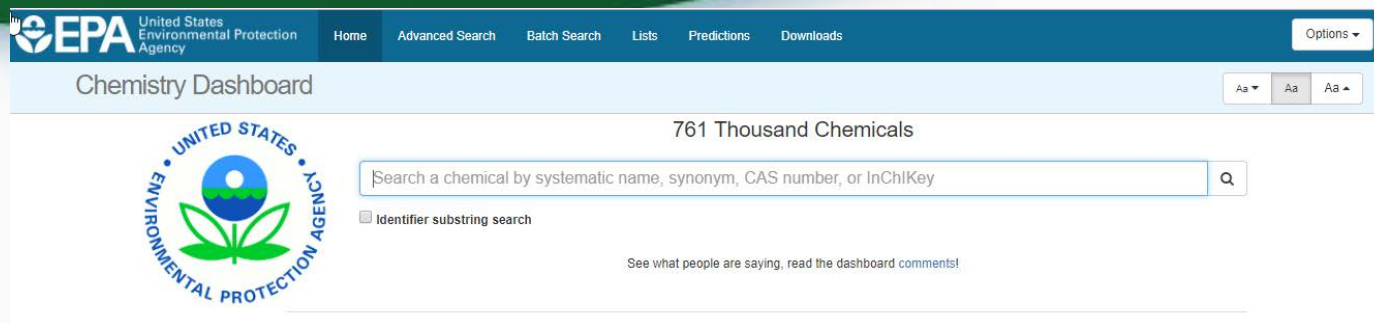
National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC

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

*March 29th 2018
Communities of Practice*

- A *very* basic intro to the dashboard
- Our latest release – Getting to What's New?
- New data and functionality
- From data to real data predictions
- Work in progress

The CompTox Chemistry Dashboard



- **A publicly accessible website** delivering access:
 - **~760,000 chemicals** with related property data
 - Experimental and predicted physicochemical property data
 - Experimental Human and Ecological hazard data
 - Integration to “biological assay data” for 1000s of chemicals
 - Information regarding consumer products containing chemicals
 - Links to other agency websites and public data resources
 - “Literature” searches for chemicals using public resources
 - “Batch searching” for thousands of chemicals
 - Real time prediction of physchem and toxicity endpoints

Williams et al. *J Cheminform* (2017) 9:61
DOI 10.1186/s13321-017-0247-6


 Journal of Cheminformatics

DATABASE

Open Access




The CompTox Chemistry Dashboard: a community data resource for environmental chemistry

Antony J. Williams^{1*} , Christopher M. Grulke¹, Jeff Edwards¹, Andrew D. McEachran², Kamel Mansouri^{1,2,4}, Nancy C. Baker³, Grace Patlewicz¹, Imran Shah¹, John F. Wambaugh¹, Richard S. Judson¹ and Ann M. Richard¹

Release Notes

https://comptox.epa.gov/dashboard/resources/comptox_release_notes.pdf




United States Environmental Protection Agency

[Home](#) [Advanced Search](#) [Batch Search](#) [Lists](#) [Predictions](#) [Downloads](#)

Chemistry Dashboard

Aa ▾ Aa Aa ▸

761 Thousand Chemicals



Identifier substring search

[See what people are saying, read the dashboard comments!](#)


Latest News

[Read more news](#)

A Major Update to the Dashboard Releases on March 7th 2018

March 7th, 2018 at 12:00:48 PM

A major update to the dashboard has been released prior to the Society of Toxicology and American Chemical Society Spring meetings. This release brings together six months of effort in adding and curating data, major updates to the batch searching functionality and access to real time predictions for both physiochemical and toxicity endpoints. [A list of release notes is available](#) for your review. We look forward to your feedback.



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- A detailed list of new functionality and fixes

** New Functionality

- * [ICD-756] - Produce link from ToxCast In Vitro Data Assay into AOP
- * [ICD-851] - Improve generation of molecular formulae
- * [ICD-929] - Include Monoisotopic Mass as Input for Batch Searching
- * [ICD-975] - Batch Search export for Batch Mass searching of MS Ready Structures
- * [ICD-977] - Add ability to download "QSAR-Ready SMILES" presently used by OPERA in the batch search
- * [ICD-1011] - Provide Download of PubMed ID and Article Title from Abstract Sifter Page
- * [ICD-1070] - Provide ability to perform batch search based on First Layer of InChIKey Only
- * [ICD-1106] - Add option to search MS-Ready Formulae or Exact Formulae
- * [ICD-1136] - Add Bioassay data plot display for selected assays
- * [ICD-1192] - Add Ranking Based on number of articles found in PubMed

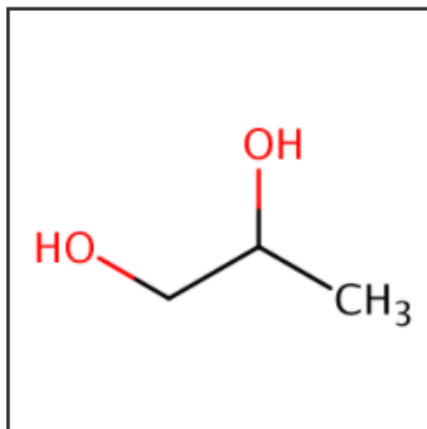
- ~3000 chemicals added since last release
- Additional experimental physchem data from literature added
- T.E.S.T predictions made across all data – physicochemical predictions
- Human and Ecological hazard data added and curated (always ongoing)
- Production volume data added

[Submit Comment](#)[Copy](#)[Aa](#)[Aa](#)[Aa](#)

1,2-Propylene glycol

57-55-6 | DTXSID0021206

© Searched by DSSTox_Substance_Id: Found 1 result for 'DTXSID0021206'.



Wikipedia

Propylene glycol (IUPAC name: propane-1,2-diol) is a synthetic organic compound with the chemical formula C₃H₈O₂. It is a viscous colorless liquid which is nearly odorless but possesses a faintly sweet taste. Chemically it is classed as a diol and is miscible with a broad range of solvents, including water, acetone, and chloroform. It is produced on a large scale and is primarily used in the production of polymers, but also sees use in food...[Read more](#)

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

[Chemical Properties](#)[Env. Fate/Transport](#)[Hazard](#)[ADME \(Beta\)](#)[Exposure](#)[Bioassays](#)[Similar Compounds](#)[Related Substances](#)[Synonyms](#)[Literature](#)[Links](#)[Comments](#)

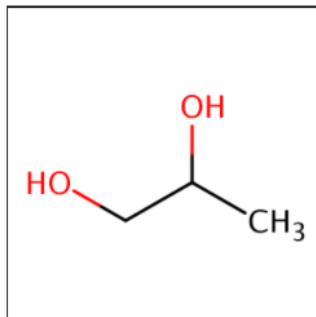
Chemistry Dashboard

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1,2-Propylene glycol

57-55-6 | DTXSID0021206

© Searched by Approved Name: Found 1 result for '1,2-propylene glycol'.



Wikipedia

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Federal

- TOX21SL: Tox21 Screening Library
- ATSDR Toxic Substances Portal Chemical List
- NIOSH International Chemical Safety Cards
- HERO: Health and Environmental Research Online
- EPA Integrated Risk Information System (IRIS)
- Provisional Peer Reviewed Toxicity Values
- EPAHFR - EPA Chemicals associated with hydraulic fracturing
- TOXCAST - EPA ToxCast Screening Library
- TOXCAST_PhaseII - EPA ToxCast Screening Library (Phase II Subset)
- TOXCAST_PhaseII - EPA ToxCast Screening Library (Phase II Subset)
- TOXCAST_ph2 - EPA ToxCast Screening Library (ph2 Subset)

US State

International

- EU Cosmetic Ingredients Inventory (Combined 2000/2006)
- KEMI List of Substances on the Market
- Pharmaceutical List with EU, Swiss and US Consumption Data

Other

- EPA Consumer Products Suspect Screening Results
- STOFF-IDENT Database of Water-Relevant Substances

Record Information

Quality Control Notes

Executive Summary (Beta) Chemical Properties Env. Fate/Transport Hazard ADME (Beta) Exposure Bioassays Similar Compounds Related Substances Synonyms Literature Links Comments

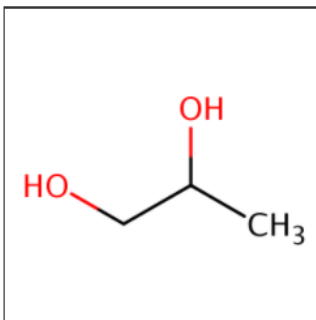
Chemistry Dashboard

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1,2-Propylene glycol

57-55-6 | DTXSID0021206

Searched by Approved Name: Found 1 result for '1,2-propylene glycol'.



Wikipedia


Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Citation 

U.S. Environmental Protection Agency, Chemistry Dashboard. <https://comptox.epa.gov/dashboard/DTXSID0021206> (accessed March 29, 2018), 1,2-Propylene glycol

Data Quality

- Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers
- Level 2: Expert curated, unique chemical identifiers using multiple sources
- Level 3: Programmatically curated from high quality EPA source, unique chemical identifiers have no conflicts in ChemID and PubChem
- Level 4: Programmatically curated from ChemID, unique chemical identifiers have no conflicts in PubChem
- Level 5: Programmatically curated from ACToR or PubChem, unique chemical identifiers with low confidence, single public source

Quality Control Notes

Executive Summary (Beta) Chemical Properties Env. Fate/Transport Hazard ADME (Beta) Exposure Bioassays Similar Compounds Related Substances Synonyms Literature Links Comments

The Executive Summary (NEW)

Chemistry Dashboard

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Executive Summary

Quantitative Risk Assessment Values

- ✗ No IRIS values
- ✓ PPRTV values available [↗](#)
- ✓ EPA RSL values available [↗](#)
- ✓ Minimum RfD: 5.0 mg/kg-day (subchronic, PPRTV (ORNL), oral, 8) [↗](#)
- ✓ Minimum RfC: 0.028 mg/m3 (subchronic, RAIS, inhalation, 7) [↗](#)
- ✗ IVIVE POD not calculated

Quantitative Hazard Values

- ✓ Minimum oral POD: 1.2e+3 mg/kg-day (developmental, COSMOS, oral, 3) [↗](#)
- ✗ No inhalation POD values
- ✓ Lowest Observed Bioactivity Equivalent Level: NR1H4

Cancer Information

- ✗ No cancer slope factor
- ✗ No inhalation unit risk value
- ✓ Carcinogenicity data available: EPA OPP cancer class: E University of Maryland carcinogenicity warning; [↗](#)
- ✗ No genotoxicity findings reported

Reproductive Toxicology

- ✓ 11 Reproductive toxicity PODs available [↗](#)

Chronic Toxicology

- ✓ 125 Chronic toxicity PODs available [↗](#)

Subchronic Toxicology

- ✓ 28 Subchronic toxicity PODs available [↗](#)

Developmental Toxicology

- ✓ 5 Developmental toxicity PODs available [↗](#)

Acute Toxicology

- ✓ 63 Acute toxicity PODs available [↗](#)

Regional Screening

Class	THQ	Value
screening level (residential Soil) (mg/kg-day)	THQ=1	1300000
screening level (residential Soil) (mg/kg-day)	THQ=0.1	130000
screening level (industrial soil) (mg/kg-day)	THQ=1	16000000
screening level (industrial soil) (mg/kg-day)	THQ=0.1	1600000
screening level (tap water) (ug/L)	THQ=1	400000
screening level (tap water) (ug/L)	THQ=0.1	40000
GIABS (mg/kg-day)	-	1
ABS (mg/kg-day)	-	0.1
risk-based SSL (mg/m3)	THQ=1	81
risk-based SSL (mg/m3)	THQ=0.1	8.1
RfDo (mg/kg-day)	-	20

The Executive Summary (NEW)

EPA United States Environmental Protection Agency Home Advanced Search Batch Search Lists Predictions Downloads Search All Data

Chemistry Dashboard

- No volatility concern.
- Biodegradation predictions are available
- BCF predictions are available
- Vapor Pressure predictions are available



logP: -0.809
log(BCF): 0.529
log(VP): -1.27

- Exposure**
 - Exposure Estimates have been predicted using the SEEM modeling methodology
- AOP Information**
 - AOP Links: 13, 16, 33, 36, 43, 58, 59, 60, 61, 66, 103, 104, 107, 124, 126, 150, 153, 163, 164, 175, 177, 187, 195, 200
- Other Notes**
 - No water quality values available.
 - 4 Air quality values available.
 - 18 Occupational exposure values available.

Point-of-Departure Plots



Oral POD: log(POD mg/kg/day)

Inhalation POD: log(POD mg/m³)

Assay Plots



EDSP: active, total (ER, AR)

ToxCast: active, total (ToxCast)

Properties, Fate and Transport

Chemistry Dashboard

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Summary

LogP: Octanol-Water

Water Solubility

Density

Flash Point

Melting Point

Boiling Point

Surface Tension

Thermal Conductivity

Vapor Pressure

Viscosity

LogKoa: Octanol-Air

Henry's Law

Index of Refraction

Molar Refractivity

Molar Volume

Download as: TSV Excel SDF

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	-0.920 (1)	-0.983 (5)	-	-0.966	-0.920	-1.34 to -0.780	-
Water Solubility	13.1 (1)	12.6 (4)	-	11.2	13.1	4.32 to 23.6	mol/L
Density	-	1.02 (2)	-	1.02	-	1.01 to 1.04	g/cm ³
Flash Point	-	88.8 (2)	-	88.8	-	70.4 to 107	°C
Melting Point	-60.0 (6)	-30.6 (4)	-60.0	-29.3	-60.0	-42.4 to -21.6	°C
Boiling Point	187 (6)	180 (5)	187	185	187 to 188	155 to 200	°C
Surface Tension	-	35.5 (2)	-	35.5	-	33.1 to 38.0	dyn/cm
Thermal Conductivity	-	185 (1)	-	-	-	-	mW/(m ² K)
Vapor Pressure	1.29e-01 (1)	1.91e-01 (4)	-	2.08e-01	1.29e-01	5.37e-02 to 2.95e-01	mmHg
Viscosity	-	12.6 (1)	-	-	-	-	cP
LogKoa: Octanol-Air	-	6.74 (1)	-	-	-	-	-
Henry's Law	-	6.02e-08 (1)	-	-	-	-	atm-m ³ /mole
Index of Refraction	-	1.43 (1)	-	-	-	-	-
Molar Refractivity	-	19.0 (1)	-	-	-	-	cm ³
Molar Volume	-	73.4 (1)	-	-	-	-	cm ³
Polarizability	-	7.52 (1)	-	-	-	-	Å ³

- When we don't have experimental data we predict it...

Property	Average		
	Experimental	Predicted	
Soil Adsorp. Coeff.	2.29 (1)	1.94 (2)	-
Atmos. Hydroxylation Rate	1.20e-11 (1)	1.30e-11 (1)	-
Biodeg. Half-Life	-	4.28 (1)	-
Fish Biotrans. Half-Life (Km)	-	8.30e-02 (1)	-
Bioaccumulation Factor	-	8.96e-01 (1)	-
Bioconcentration Factor	-	2.13 (5)	-

Mansouri et al. *J Cheminform* (2018) 10:10
<https://doi.org/10.1186/s13321-018-0263-1>


 Journal of Cheminformatics

RESEARCH ARTICLE

Open Access



OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri^{1,2,3*} , Chris M. Grulke¹, Richard S. Judson¹ and Antony J. Williams¹

Model Performance Details

(Redesigned display)

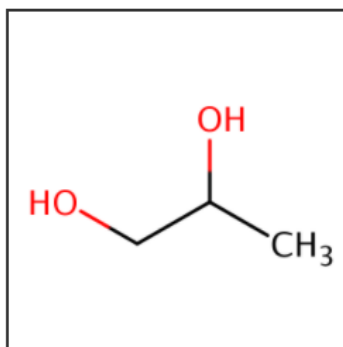
Chemistry Dashboard

OPERA Models: Fish Biotrans. Half-Life (Km)

1,2-Propylene glycol

57-55-6 | DTXSID0021206

Save PDF



Model Results

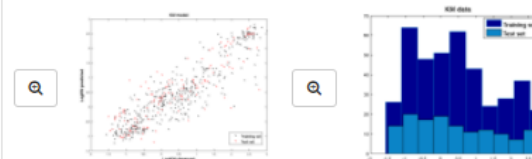
Predicted value: 8.30e-02 days

Global applicability domain: **Inside**

Local applicability domain index: 0.28

Confidence level: 0.71

Model Performance



Weighted KNN model

QMRF

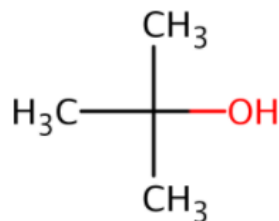
5-fold CV (75%)

Training (75%)

Test (25%)

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.83	0.49	0.82	0.5	0.73	0.62

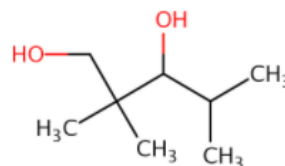
Nearest Neighbors from the Training Set



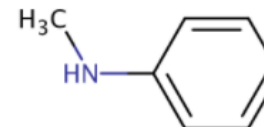
tert-Butyl alcohol
Measured: 7.41e-02
Predicted: 7.66e-02



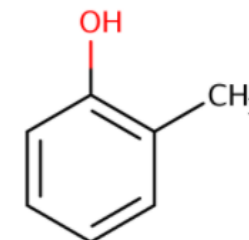
Pentaerythritol dibromide
Measured: 3.98e-02
Predicted: 5.44e-02



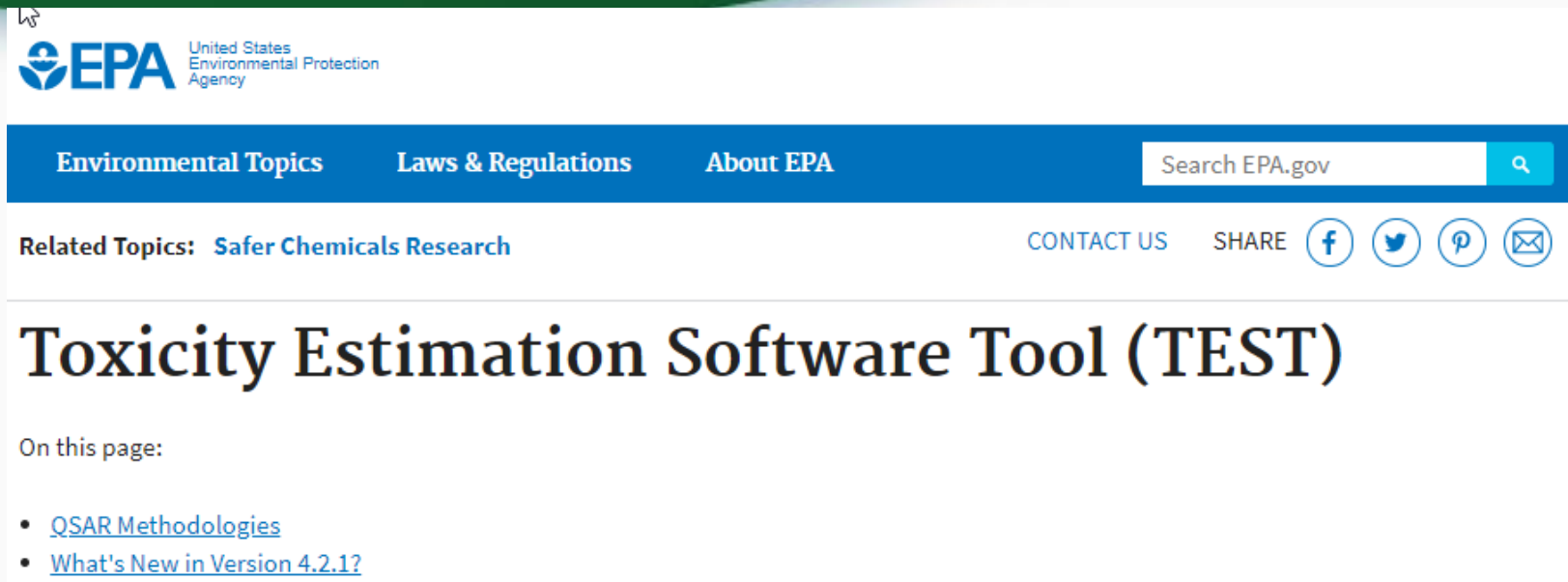
2,2,4-Trimethyl-1,3-pentanediol
Measured: 4.57e-02
Predicted: 5.13e-02



N-Methylaniline
Measured: 1.32e-01
Predicted: 1.50e-01



o-Cresol
Measured: 3.02e-01
Predicted: 2.42e-01



The screenshot shows the EPA website header with the EPA logo and navigation links: Environmental Topics, Laws & Regulations, and About EPA. A search bar is present with the text "Search EPA.gov". Below the navigation is a "Related Topics" section with a link to "Safer Chemicals Research". On the right side, there are links for "CONTACT US" and "SHARE" with social media icons for Facebook, Twitter, Pinterest, and Email. The main heading is "Toxicity Estimation Software Tool (TEST)". Underneath, it says "On this page:" followed by two bullet points: "[QSAR Methodologies](#)" and "[What's New in Version 4.2.1?](#)".

- Predictions made for the whole database
- Includes detailed calculation reports

T.E.S.T Calculation Reports

Chemistry Dashboard Search All Data

Predicted Water solubility at 25°C for 57-55-6 from Consensus method Download PDF


Prediction results

Endpoint	Experimental value (CAS# 57-55-6) Source: EPI Suite v 4.05	Predicted value ^a
Water solubility at 25°C (-log10(mol/L))	-1.12	-0.64
Water solubility at 25°C mg/L	1001017.62	226641.67

^aNote: the test chemical was present in the training set. The prediction does not represent an external prediction.

Individual Predictions

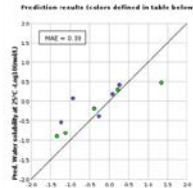
Method	Predicted value (-Log10(mol/L))
Hierarchical clustering	-1.12
Group contribution	0.01
Nearest neighbor	-0.80





Predictions for the test chemical and for the most similar chemicals in the external test set
 If the predicted value matches the experimental values for similar chemicals in the test set (and the similar chemicals were predicted well), one has greater confidence in the predicted value.

Chemicals	MAE ^b
Entire set	0.56
Similarity coefficient > 0.5	0.29

^bMean absolute error in -Log10(mol/L)



CAS	Structure	Similarity Coefficient	Experimental value -Log10(mol/L)	Predicted value -Log10(mol/L)
57-55-6 (test chemical)			-1.12	-0.64
78-92-2		0.96	-0.39	-0.18
64-17-5		0.95	-1.34	-0.91
584-02-1		0.92	0.23	0.30
353-36-6		0.91	1.35	0.48
109-86-4		0.90	-1.12	-0.82

Access to Chemical Hazard Data

Chemistry Dashboard | EPAHFR

Submit Comment Copy Aa Aa Aa

- Chemical Properties
- Env. Fate/Transport
- Hazard
- ADME (Beta)
- Exposure
- Bioassays
- Similar Compounds
- Related Substances
- Synonyms
- Literature
- Links
- Comments

- Exposure Limit
- Lethality Effect Level
- Point of Departure**
- Toxicity Value

Download table as: TSV Excel **Human** Eco

Risk Assessment

Download as: TSV Excel

Study ID	reference value type	screening value	reference value	reference value units	study type	tissue	endpoint	POD	POD units	POD type	benchmark response	IRIS flag	uncertainty factor A	uncertainty factor D	uncertainty factor H	uncertainty factor
16000009	Sub-chronic Reference Dose (s-RfD)	0	20	mg/kg bw-day ADD	Sub-chronic	Hematologic	Erythrocyte count (RBC)	5200	mg/kg bw-day ADD	LOAEL		0	10	1	10	3
16000009	Chronic Reference Dose (c-RfD)	0	20	mg/kg bw-day ADD	Sub-chronic	Hematologic	Erythrocyte count (RBC)	5200	mg/kg bw-day ADD	LOAEL		0	10	1	10	3

Close

In Vitro Bioassay Screening

ToxCast and Tox21

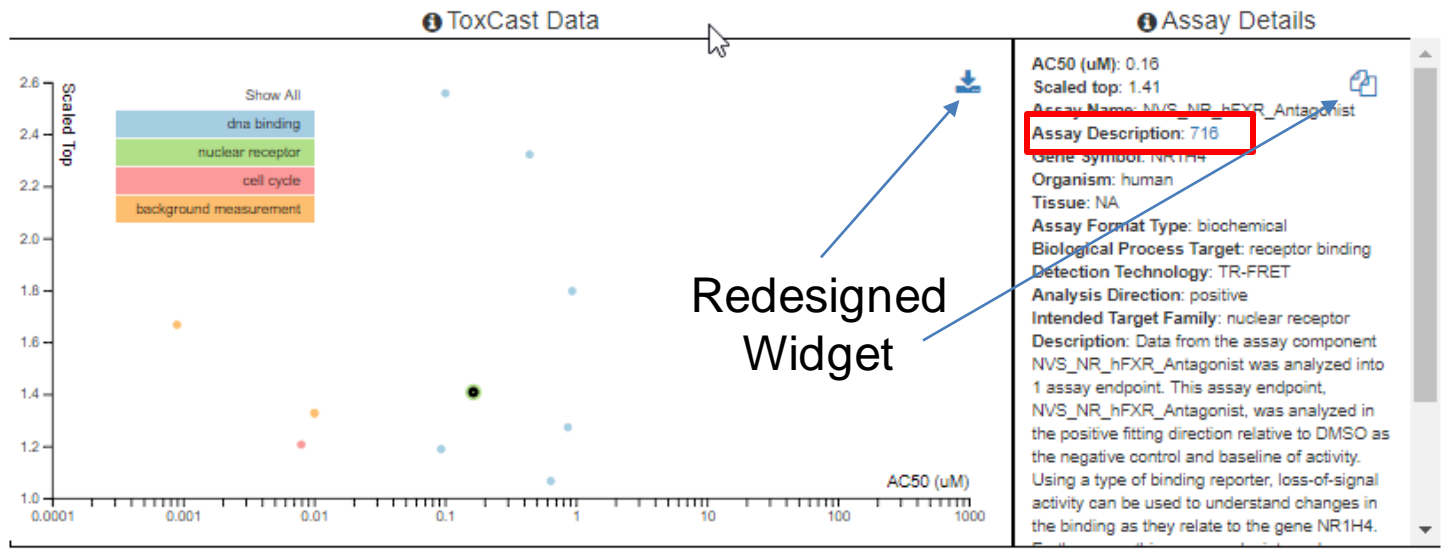
Chemistry Dashboard | EPAHFR

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- Chemical Properties
- Env. Fate/Transport
- Hazard
- ADME (Beta)
- Exposure
- Bioassays
- Similar Compounds
- Related Substances
- Synonyms
- Literature
- Links
- Comments

ToxCast: Summary
PubChem

Chemical Activity Summary



Redesigned Widget

Download as: TSV Excel Show: Inactive Background

Assay Name Assa... SeqA... AOP Link AOP Eve... Hit Call T... Scale... log ... Target Family

Detailed Assay Description as PDF (limited number of assays)

NVS_NR_hFXR_Antagonist

Assay Title: NovaScreen Human Farnesoid x Receptor Alpha (FXR) Ligand-Binding Antagonist Screening Assay

1. Assay Descriptions

1.1. Overview

Assay Summary:

High-throughput screening of in vitro chemical-target interactions across a wide variety of compounds through a broad range of biochemical interactions will help describe the chemical-assay bioactivity space for chemicals with limited available information. There exists a large number of environmental chemicals for which there is little information about the potential for bioactivity. The NVS NR human farnesoid x receptor (FXR, NR1H4) agonist assay format allows for an efficient screening of thousands of chemicals for the ability to competitively bind to the ligand-binding domain of a xenobiotic sensing nuclear receptor. This assay was developed to screen the ToxCast chemical library for potential farnesoid x receptor ligand-binding activity using a TR-FRET competitive displacement assay and a known FXR receptor agonist (Chenodeoxycholic Acid, CDCA) as a reference compound. Biochemical high-throughput screening offers preliminary evidence for chemical targets in a cell or tissues which, when combined with information from literature or targeted in vivo studies, can indicate potential pathways for toxicity. This assay was run for a test duration of 1 hour in a 384-well plate.

1.2. Assay Definition

Assay Throughput:

Human FXR ligand-binding domain (LBD) incubated in 384-well microtiter plates for 1 hour prior to measuring ligand dependent binding of cofactor to the receptor using TR-FRET.

Sources of Exposure to Chemicals

Exposure [Bioassays](#) [Similar Compounds](#) [Related Substances](#) [Synonyms](#) [Literature](#) [Links](#) [Comments](#)

Product & Use Categories

Chemical Weight Fraction

Chemical Functional Use

Monitoring Data


Exposure Predictions

Production Volume

Product & Use Categories (PUCs)

Categorization type	Number of Unique Products
PUC	288
PUC	208
PUC	117
PUC	107
PUC	107
PUC	101
PUC	101
PUC	90
PUC	89

Related Substances Mappings to Transformation Products

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Search All Data

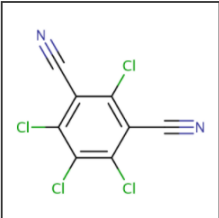
Chemistry Dashboard

Submit Comment Share Copy As As As

Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by Approved Name: Found 1 result for 'Chlorothalonil'.



Wikipedia

Chlorothalonil (2,4,5,6-tetrachloroisophthalonitrile) is an organic compound mainly used as a broad spectrum, nonsystemic fungicide, with other uses as a wood preservative, pesticide, acaricide, and to control mold, mildew, bacteria, algae. Chlorothalonil-containing products are sold under the names Bravo, Echo, and Daconil. It was first registered for use in the US in 1905. In 1997, the most recent year for which data are available, it was the third most used fungicide in the US, behind... [Read more](#)

Intrinsic Properties

Structural Identifiers

Linked Substances

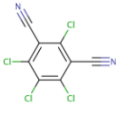
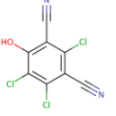
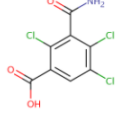
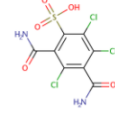
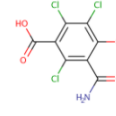
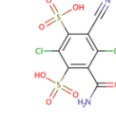
Presence in Lists

Record Information

Quality Control Notes

Executive Summary (Beta) Chemical Properties Env. Fate/Transport Hazard ADME (Beta) Exposure Bioassays Similar Compounds **Related Substances** Synonyms Literature Links Comments

Download / Send Sort by: Relationship 8 chemicals Hide: Select all

Searched Chemical	Transformation Product	Transformation Product	Transformation Product	Transformation Product	Transformation Product
 Chlorothalonil 1897-45-6	 4-Hydroxy-2,5,6-trichloroisophthalonitrile 28343-61-5	 3-Carbamoyl-2,4,5-trichlorobenzoic acid 142733-37-7	 2,4-dicarbamoyl-3,5,6-trichlorobenzene... NOCAS_891327	 3-carbamoyl-2,5,6-trichloro-4-hydroxybenzoic acid... NOCAS_891328	 4-carbamoyl-2,5-dichloro-6-cyanobenzamide... NOCAS_891329

Identifiers to Support Searches

Chemical Properties

Env. Fate/Transport

Hazard

ADME (Beta)

Exposure

Bioassays


Similar Compounds

Related Substances

Synonyms

Found 78 synonyms

Legend: **Valid Synonyms** *Good Synonyms* *Other Synonyms*

 Copy all Synonyms

1,2-Propylene glycol

Propane-1,2-diol

1,2-Propanediol

57-55-6 Active CAS-RN

alpha-Propylene glycol

(+/-) 1,2-Propanediol

(RS)-1,2-Propanediol

dl-Propylene glycol

3-01-00-02142 Beilstein Registry Number

1,2-Propanediol

(+/-)-1,2-Propanediol

(+/-)-Propylene glycol

1,2-(RS)-Propanediol

1,2-DIHYDROXYPROPANE

1,2-PROPANDIOL

Literature Searches and Links

[Chemical Properties](#)
[Env. Fate/Transport](#)
[Hazard](#)
[ADME \(Beta\)](#)
[Exposure](#)
[Bioassays](#)
[Similar Compounds](#)
[Related Substances](#)
[Synonyms](#)
[Literature](#)
[Links](#)
[Comments](#)

[Google Scholar](#)
[PubMed Abstract Sifter](#)
[PubChem Articles](#)
[PubChem Patents](#)
[PPRTV](#)
[IRIS](#)

1) Select PubMed starting point query then 2) click on Retrieve. **i**

Hazard **i**

Optionally, edit the query before retrieving.

("57-55-8" OR "1,2-Propylene glycol" OR "Propylene Glycol") AND (NOAEL OR NOEL OR LOEL OR Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

13 of 13 articles loaded...

To find articles quickly, enter terms to sift abstracts. **i**

[Download / Send to...](#)
[Download Sifter for Excel](#)

<input type="checkbox"/>	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	27101543	2016	Electronic cigarettes: a systematic review of available studies on hea...	Zulkifli; Abidin; Abidin; Amer Nordin; Praveena; Sye...	Reviews on environmental health	
<input type="checkbox"/>	26787428	2016	Toxicological assessment of a prototype e-cigaret device and three fl...	Werley; Kirkpatrick; Oldham; Jerome; Langston; Lill...	Inhalation toxicology	
<input type="checkbox"/>	26475513	2015	Deriving Biomonitoring Equivalents for selected E- and P-series glyco...	Poet; Ball; Hays	International journal of hygiene and environmental h...	
<input type="checkbox"/>	26120296	2015	Potential harmful health effects of inhaling nicotine-free shisha-pen v...	Kienhuis; Soeteman-Hernandez; Bos; Cremers; Kle...	Tobacco induced diseases	
<input type="checkbox"/>	25527861	2014	Efinaconazole: Developmental and reproductive toxicity potential of ...	Glynn; Jo; Minowa; Sanada; Nejishima; Matsuuchi; ...	Reproductive toxicology (Elmsford, N.Y.)	
<input type="checkbox"/>	25038564	2014	Nonclinical safety assessment of Efinaconazole Solution (10%) for o...	Jo; Glynn; Nejishima; Sanada; Minowa; Calvarese; ...	Regulatory toxicology and pharmacology : RTP	
<input type="checkbox"/>	24138296	2013	Solvent-based formulations for intravenous mouse pharmacokinetic ...	Thackaberry; Wang; Schweiger; Messick; Valle; De...	Xenobiotica: the fate of foreign compounds in biolog...	
<input type="checkbox"/>	21683116	2011	Non-clinical safety and pharmacokinetic evaluations of propylene gly...	Werley; McDonald; Lilly; Kirkpatrick; Wallery; Byron;...	Toxicology	
<input type="checkbox"/>	18830862	2008	Final report on the safety assessment of methoxyisopropanol and m...		International journal of toxicology	
<input type="checkbox"/>	15876203	2005	Using physiologically-based pharmacokinetic modeling to address n...	Kiman; Sweeney; Corley; Gargas	Risk analysis : an official publication of the Society f...	
<input type="checkbox"/>	12583407	2003	Significance of 2-methoxypropionic acid formed from beta-propylene...	Carney; Pottenger; Johnson; Liberacki; Tomesi; Dry...	Toxicological sciences : an official journal of the Soc...	

ptox.zn.epa.gov/dashboard/dsstoxdb/results





Check for updates

SOFTWARE TOOL ARTICLE

Abstract Sifter: a comprehensive front-end system to PubMed

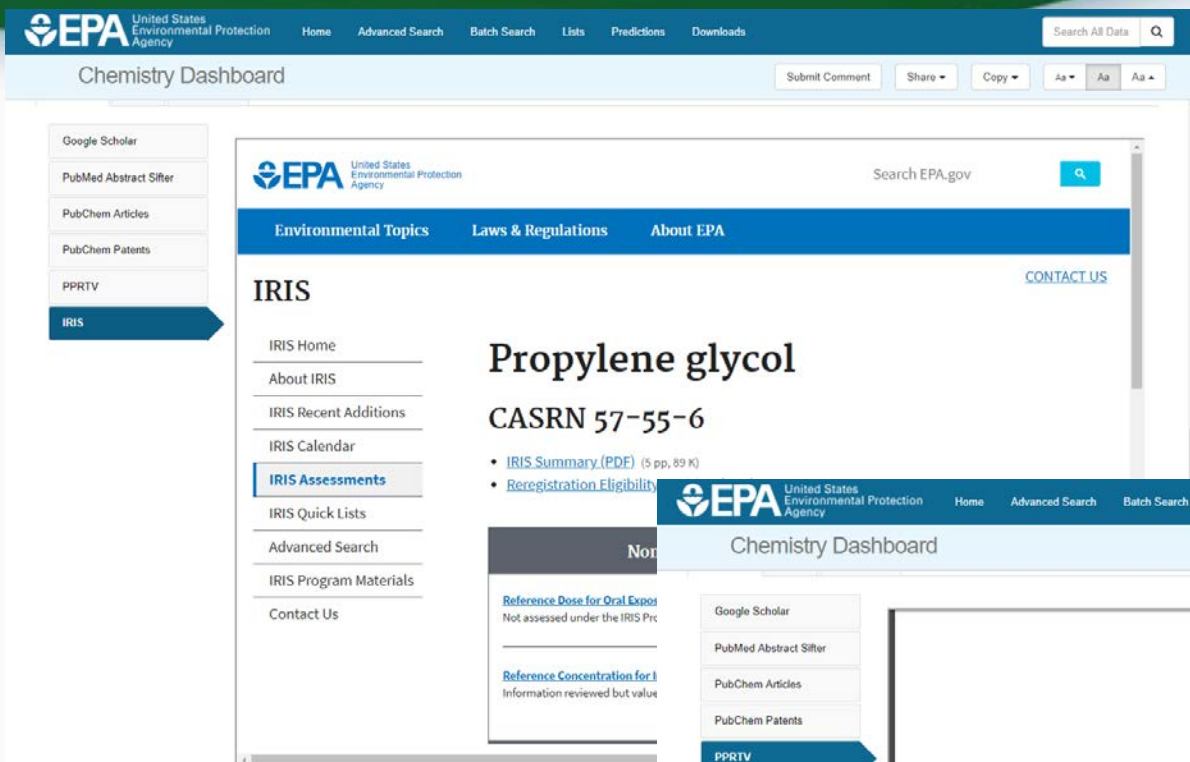
[version 1; referees: 2 approved]

Nancy Baker ¹, Thomas Knudsen², Antony Williams ²

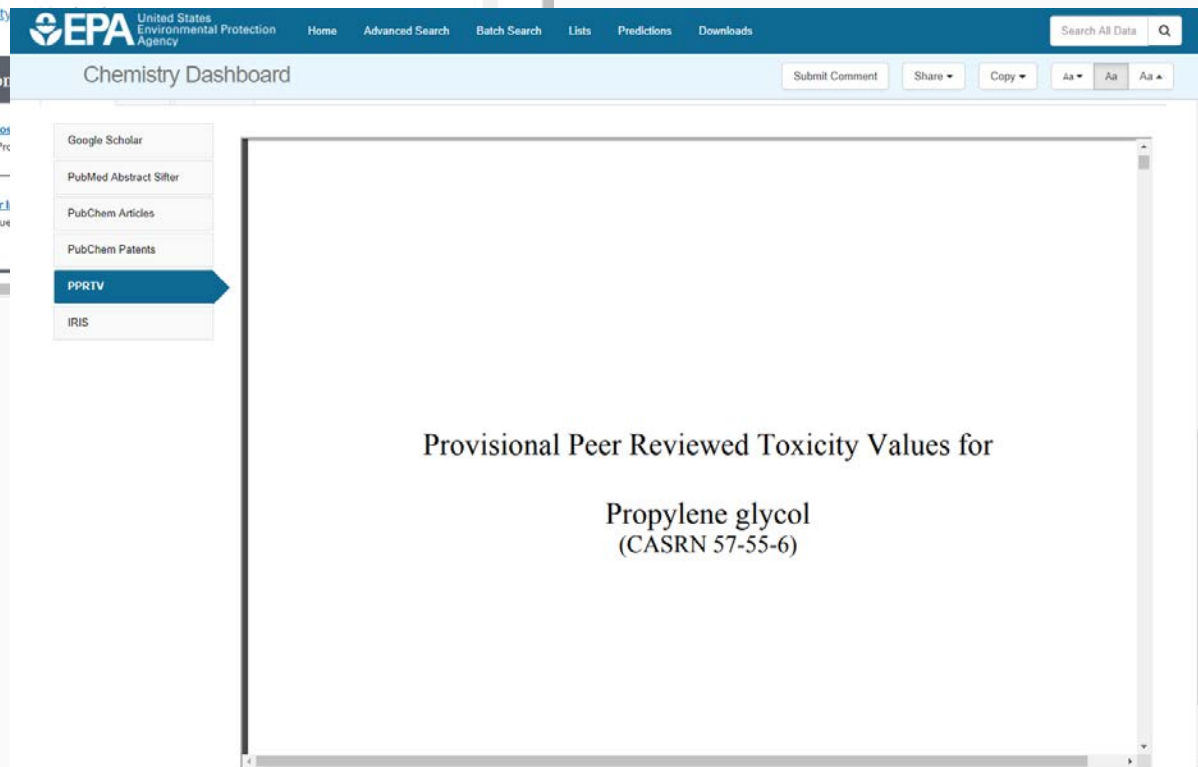
¹Leidos, Research Triangle Park, NC, USA

²National Center for Computational Toxicology, U.S. Environmental Protection Agency, Research Triangle Park, NC, USA

Links to PPRTV and IRIS



The screenshot shows the EPA Chemistry Dashboard interface. The top navigation bar includes the EPA logo, "United States Environmental Protection Agency", and links for Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. A search bar labeled "Search All Data" is on the right. Below the navigation bar, the page title "Chemistry Dashboard" is displayed, along with "Submit Comment", "Share", "Copy", and font size controls. On the left, a sidebar menu lists various search options: Google Scholar, PubMed Abstract Sifter, PubChem Articles, PubChem Patents, PPRTV, and IRIS (which is highlighted with a blue arrow). The main content area features the EPA logo and "Search EPA.gov" at the top. Below this is a blue navigation bar with "Environmental Topics", "Laws & Regulations", and "About EPA", and a "CONTACT US" link. The main heading is "IRIS", with a sub-heading "Propylene glycol" and "CASRN 57-55-6". A list of links includes "IRIS Summary (PDE) (5 pp, 89 K)" and "Registration Eligibility". Below the heading, there is a "Not" section with two links: "Reference Dose for Oral Exposure" (with subtext "Not assessed under the IRIS Process") and "Reference Concentration for Inhalation" (with subtext "Information reviewed but values not available").



The screenshot shows the EPA Chemistry Dashboard interface for the PPRTV page. The top navigation bar is identical to the previous screenshot. The main heading is "PPRTV" (highlighted with a blue arrow in the sidebar) and "Propylene glycol (CASRN 57-55-6)". The central text reads "Provisional Peer Reviewed Toxicity Values for Propylene glycol (CASRN 57-55-6)". The sidebar menu on the left lists: Google Scholar, PubMed Abstract Sifter, PubChem Articles, PubChem Patents, PPRTV (highlighted with a blue arrow), and IRIS.

External Links to Data and Services

WS

Chemical Properties

Env. Fate/Transport

Hazard

ADME (Beta)

Exposure

Bioassays

Similar Compounds
















Related Substances

Synonyms















Literature

Links
















General

-  EPA Substance Registry ...
-  Household Products Data...
-  PubChem
-  CPCat
-  DrugBank
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  Chemical Vendors
-  NIOSH Chemical Safety ...
-  ToxPlanet
-  ACS Reagent Chemicals
-  Wikidata
-  ChemHat: Hazards and A...
-  Wolfram Alpha

Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  eChemPortal
-  Gene-Tox
-  HSDB
-  ToxCast Dashboard 2
-  LactMed
-  International Toxicity Esti...
-  ATSDR Toxic Substances...
-  ACToR PDF Report
-  CREST






Publications

-  Toxline
-  Environmental Health Per...
-  NIEHS
-  National Toxicology Progr...
-  Google Books
-  Google Scholar
-  Google Patents
-  PPRTVWEB
-  PubMed
-  IRIS Assessments
-  EPA HERO
-  RSC Publications
-  BioCaddie DataMed
-  Springer Materials
-  Federal Register

Analytical

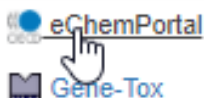
-  RSC Analytical Abstracts
-  Tox21 Analytical Data
-  MONA: MassBank North ...
-  NIST NIST IR Spectrum
-  NIST NIST MS Spectrum

Prediction

-  2D NMR HSQC/HMBC Pr...
-  Carbon-13 NMR Prediction
-  Proton NMR Prediction
-  ChemRTP Predictor
-  LSERD

Integrated Linkouts

eChemPortal provides free public access to information on properties of chemicals. Direct links to collections of chemical hazard and risk information prepared for government chemical review programmes at national, regional and international levels are obtained.



The International Chemical Safety Cards (ICSC) summarize essential health and safety information on chemicals for their use at the

[NIOSH Chemical Safety ...](#)

Comparative Toxicogenomics Database is a robust, publicly available database that aims to advance understanding about how environmental exposures affect human health.



Integrated Linkouts

Comparative Toxicogenomics DB

Comparative Toxicogenomics Database

Propylene Glycol

These diseases are associated with *Propylene Glycol* or its descendants. Each association is *curated* (M marker/mechanism and/or T therapeutic) and/or *inferred* (via a curated gene interaction).

Disease categories [\[Show chart\]](#)



Filter by Disease category: ALL Association type: ALL Filter

1-50 of 240 results. First Previous 1 2 3 4 5 Next Last

	Chemical	Disease	Direct Evidence	Enrichment Analysis	Inference Network	Inference Score	References
1.	Propylene Glycol	Drug-Related Side Effects and Adverse Reactions	M	GO	2 genes: ABCC2 ABCC4	4.09	5
2.	Propylene Glycol	Acute Kidney Injury	M	GO	2 genes: IL6 TGFB1	3.78	3
3.	Propylene Glycol	Chemical and Drug Induced Liver Injury	M	GO	2 genes: ABCC2 IL6	2.82	5
4.	Propylene Glycol	Kidney Diseases	M		1 gene: TGFB1	2.54	4

Advanced Search

Mass Search

Min/Max ▼

Da Da ppm

Molecular Formula Search

MS Ready Formula 
 Exact Formula 

Generate Molecular Formula(e)

Min/Max

Da Da ppm

Default Options: C[1-50] H[0-100] O[0-20] N[0-20] P[0-20] S[0-10]

Include Halogens: F[0-20] Cl[0-20] Br[0-20] I[0-20]

Options ▼

Advanced Searches


Mass Based Search

Mass Search

Min/Max

Da

Advanced Searches


 United States Environmental Protection Agency


Home Advanced Search Batch Search Lists Predictions Downloads

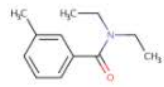
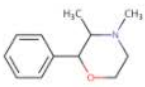
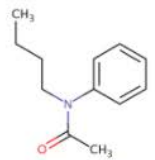
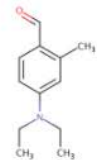
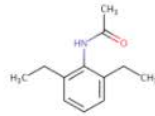
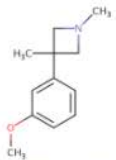
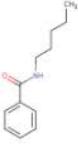
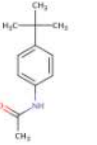
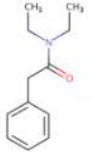
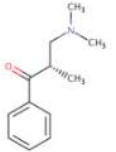
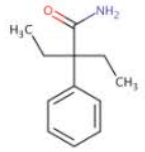
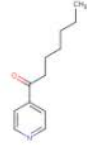
Search All Data

Chemistry Dashboard

Search Results
Searched by Mass: '191.031 +/- 5 ppm'.
298 of 298 chemicals visible

Download / Send Sort by: Mass Difference 

Hide: **Multicomponent Chemicals** 

 <p>DEET 134-62-3</p>	 <p>Phendimetrazine 634-03-7</p>	 <p>N-Butylacetanilide 91-49-6</p>	 <p>Benzaldehyde, 4-(diethylamino)-... 92-14-8</p>	 <p>Acetanilide, 2,6-diethyl- 16665-89-7</p>	 <p>Azetidine, 1,3-dimethyl-3-(m-met... 19832-26-9</p>
 <p>Benzamide, N-pentyl- 20308-43-4</p>	 <p>p-t-Butylacetanilide 20330-45-4</p>	 <p>N,N-Diethylphenylacetamide 2431-96-1</p>	 <p>3-(Dimethylamino)-2-methylpropi... 26171-50-6</p>	 <p>Butyramide, 2-ethyl-2-phenyl- 30568-39-9</p>	 <p>1-Heptanone, 1-(4-pyridyl)- 32941-30-3</p>

The Dashboard to Support MS-Analysis

Mass Search ⓘ

▼

Da

Molecular Formula Search ⓘ

MS Ready Formula ⓘ
 Exact Formula ⓘ

Generate Molecular Formula(e) ⓘ

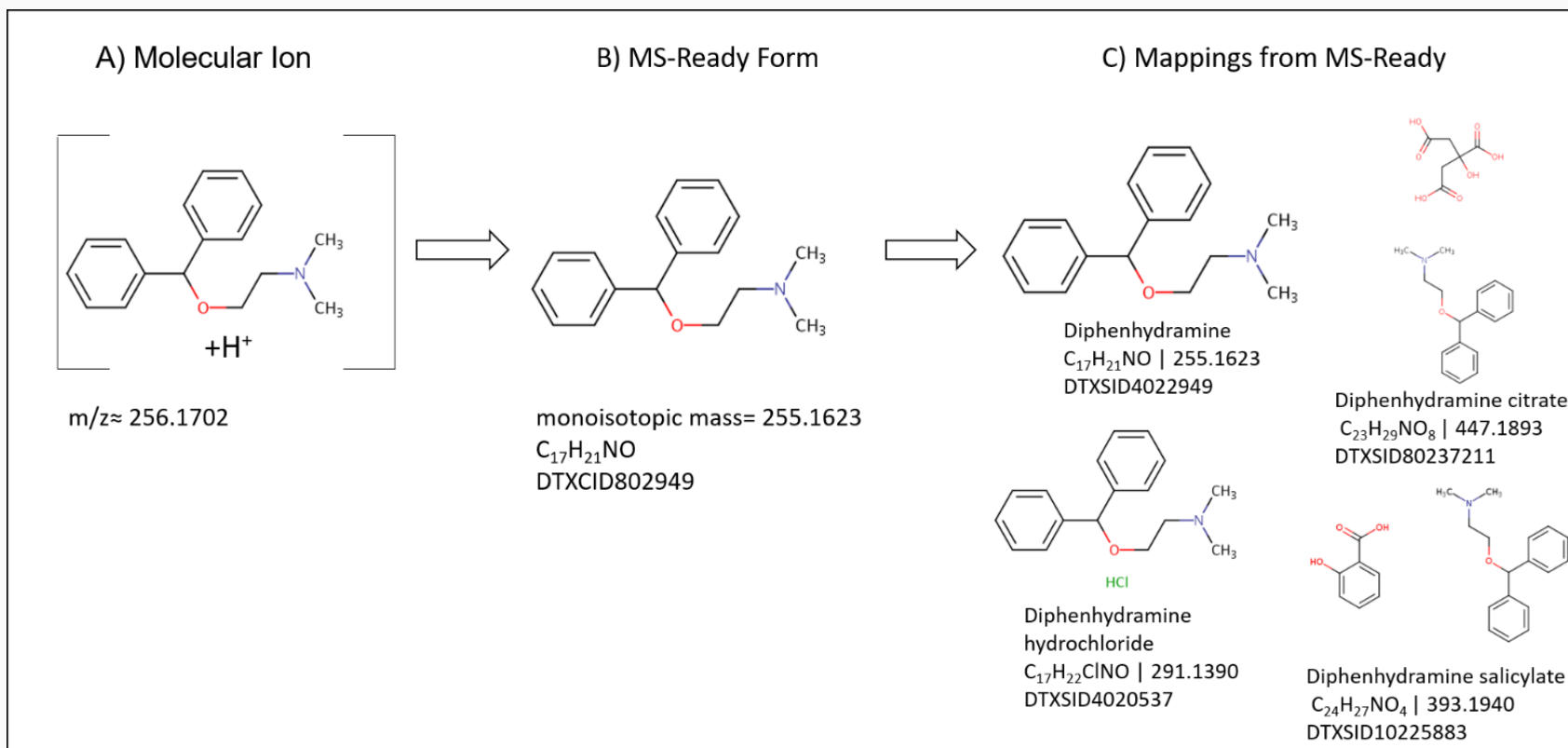
Da

Default Options: C[1-50] H[0-100] O[0-20] N[0-20] P[0-20] S[0-10]
Include Halogens: F[0-20] Cl[0-20] Br[0-20] I[0-20]

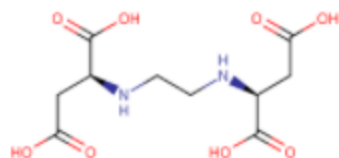
Options ▼

MS-Ready Structures Underpin Analysis

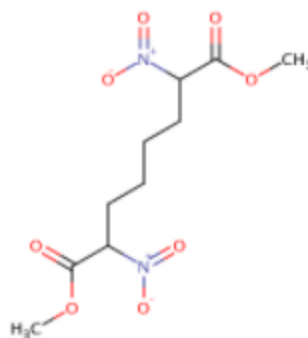
Specific Data-Mappings “MS-Ready Structures”



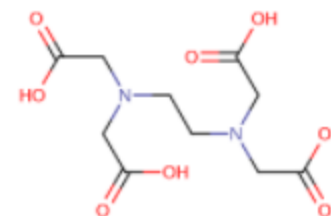
- Input Formula: C₁₀H₁₆N₂O₈
- EXACT Formula Search: 3 Chemicals



N,N'-Ethylenedi-L-aspartic acid
20846-91-7



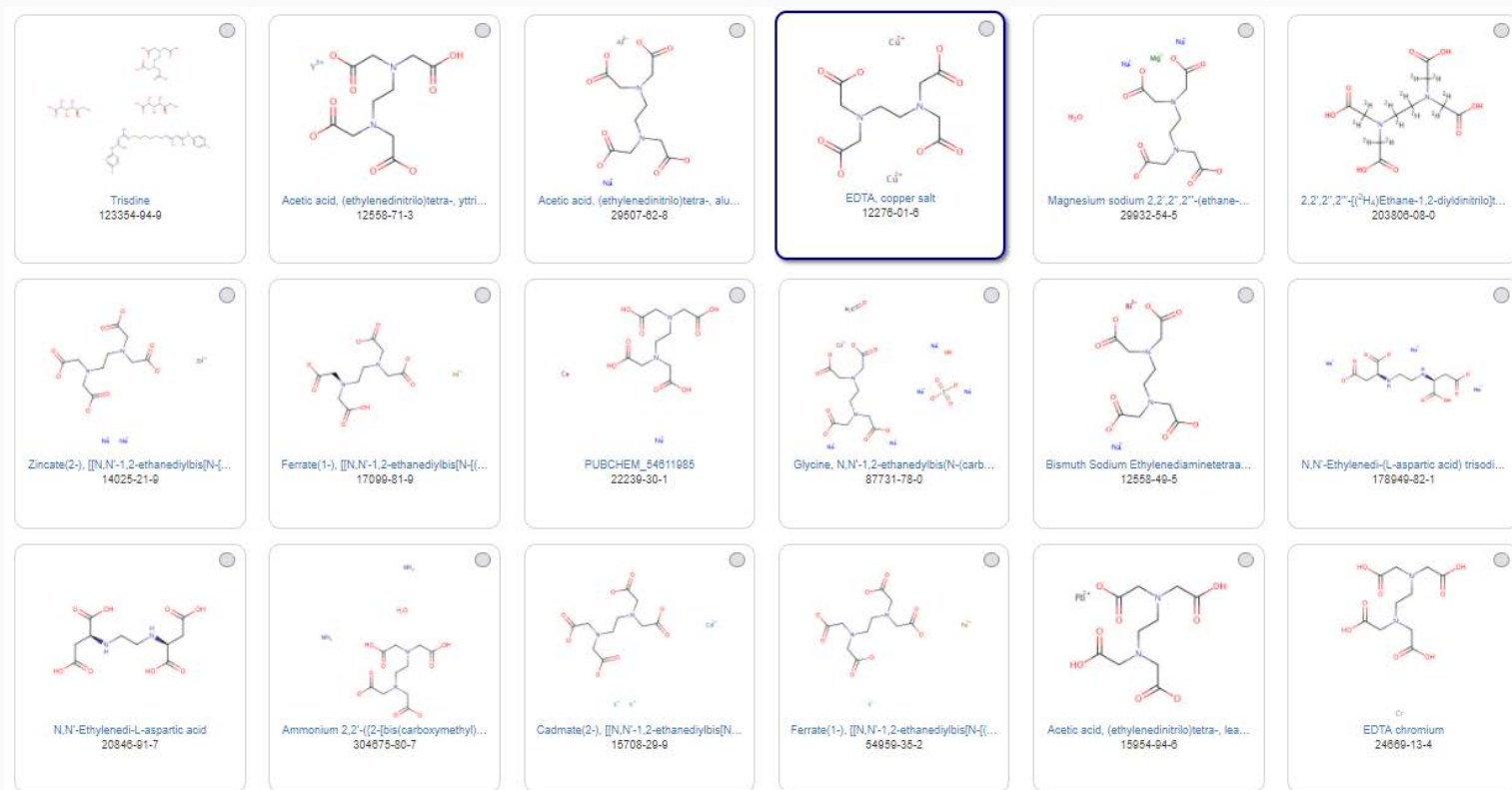
Dimethyl 2,7-dinitrooctanedioate
67404-09-5



Ethylenediaminetetraacetic acid
60-00-4

MS-Ready Mappings


- **Same Input Formula: C₁₀H₁₆N₂O₈**
- **MS Ready Formula Search: 88 Chemicals**










Batch Searches

Batch Search



Please enter one identifier per line 

Select Input Type(s)

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





Enter Identifiers to Search (searches should be limited to <1000 identifiers)

```
1445-75-6
50-00-0
107-06-2
57-12-5
7550-45-0
79-01-6
121-82-4
108-05-4
7803-51-2
122-66-7
```









Display All Chemicals

Download Chemical Data

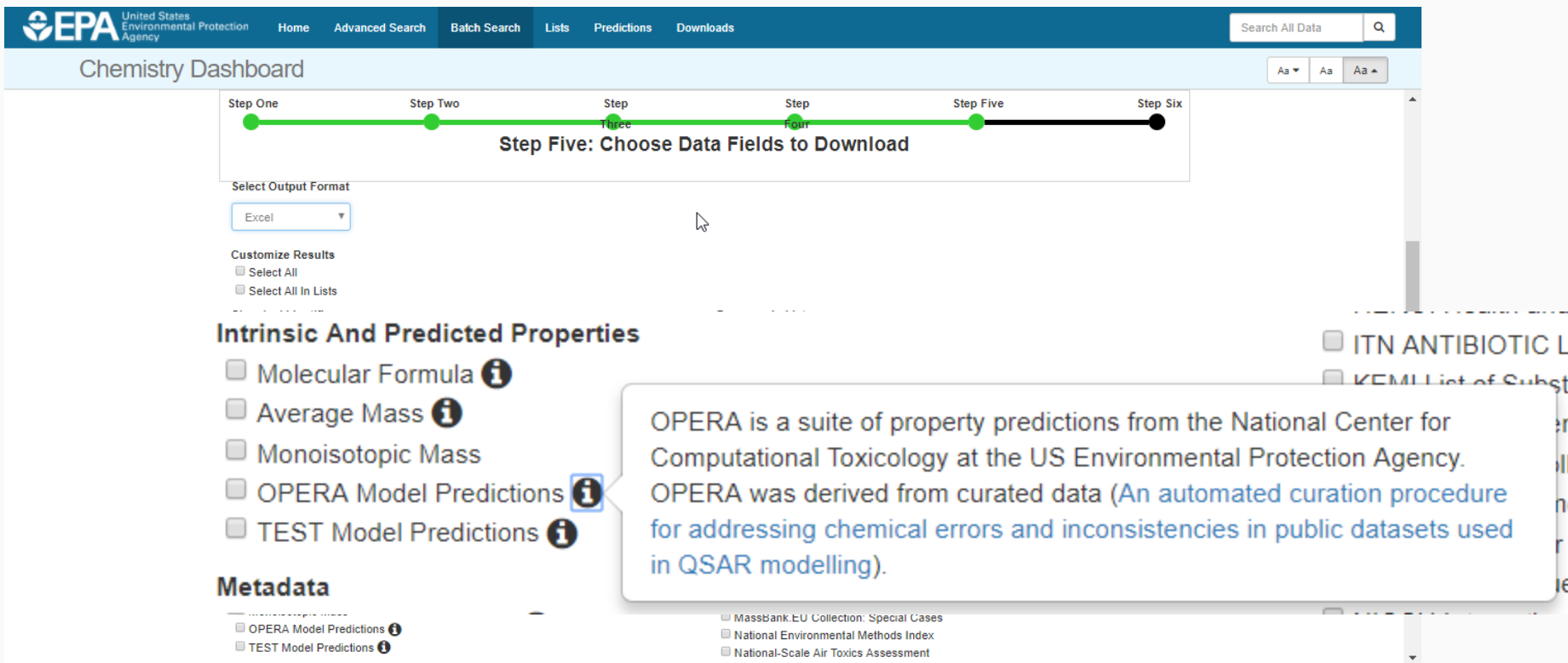
Intrinsic And Predicted Properties

- Molecular Formula 
- Average Mass 
- Monoisotopic Mass
- OPERA Model Predictions 
- TEST Model Predictions 

Metadata

- Curation Level Details 
- Data Sources 
- Assay Hit Count 
- Include links to ACToR reports - SLOW! (BETA) 
- NHANES/Predicted Exposure 
- Include ToxVal Data Availability 
- Number of PubMed Articles 
- Abstract Sifter Input File (Beta) 
- MetFrag Input File(Beta)
- IRIS
- PPRTV
- PubChem Data Sources

OPERA and TEST in Batch



The screenshot displays the EPA Chemistry Dashboard interface. At the top, there is a navigation bar with the EPA logo and menu items: Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. A search bar labeled 'Search All Data' is on the right. Below the navigation bar is the 'Chemistry Dashboard' header with a search bar and font size controls. A progress bar at the top shows six steps, with Step Five highlighted and labeled 'Step Five: Choose Data Fields to Download'. Below the progress bar, the 'Select Output Format' dropdown is set to 'Excel'. Under 'Customize Results', there are checkboxes for 'Select All' and 'Select All In Lists'. The main content area is divided into sections: 'Intrinsic And Predicted Properties' with checkboxes for Molecular Formula, Average Mass, Monoisotopic Mass, OPERA Model Predictions, and TEST Model Predictions; and 'Metadata' with checkboxes for OPERA Model Predictions, TEST Model Predictions, MassBank.EU Collection: Special Cases, National Environmental Methods Index, and National-Scale Air Toxics Assessment. A callout box on the right contains text about OPERA.

Step Five: Choose Data Fields to Download

Select Output Format: Excel

Customize Results

- Select All
- Select All In Lists

Intrinsic And Predicted Properties


- Molecular Formula **i**
- Average Mass **i**
- Monoisotopic Mass
- OPERA Model Predictions **i**
- TEST Model Predictions **i**

Metadata

- OPERA Model Predictions **i**
- TEST Model Predictions **i**
- MassBank.EU Collection: Special Cases
- National Environmental Methods Index
- National-Scale Air Toxics Assessment

OPERA is a suite of property predictions from the National Center for Computational Toxicology at the US Environmental Protection Agency. OPERA was derived from curated data (An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling).






Select Output Format

Excel 



Customize Results

- Select All
- Select All In Lists






Chemical Identifiers

- DTXSID 
- Chemical Name 
- CAS-RN 
- InChIKey 
- IUPAC Name 
- Synonyms and Identifiers









Structures

- Mol File 
- SMILES 
- InChI String 

Intrinsic And Predicted Properties

- Molecular Formula 
- Average Mass 
- Monoisotopic Mass 
- OPERA Model Predictions 
- TEST Model Predictions 

Metadata

- Curation Level Details 
- Data Sources 
- Assay Hit Count 
- Include links to ACToR reports - SLOW! (BETA) 
- NHANES/Predicted Exposure 
- Include ToxVal Data Availability 
- Number of PubMed Articles 
- Abstract Sifter Input File (Beta) 
- MetFrag Input File(Beta)
- IRIS
- PPRTV
- PubChem Data Sources


Excel Output

	A	B	C	D	E	F	G	H
1	INPUT	FOUND_BY	DTXSID	PREFERRED_NAME	EXPOCAST	EXPOCAST	NHANES	TOXVAL_D
2	1445-75-6	CAS-RN	DTXSID5024051	Diisopropyl methylphos	2.09e-08	Y	-	Y
3	50-00-0	CAS-RN	DTXSID7020637	Formaldehyde	1.32e-06	Y	-	Y
4	107-06-2	CAS-RN	DTXSID6020438	1,2-Dichloroethane	4.9e-06	Y	-	Y
5	57-12-5	CAS-RN	DTXSID6023991	Cyanide	-	-	-	Y
6	7550-45-0	CAS-RN	DTXSID8042476	Titanium tetrachloride	-	-	-	Y
7	79-01-6	CAS-RN	DTXSID0021383	Trichloroethylene	7.27e-06	Y	-	Y
8	121-82-4	CAS-RN	DTXSID9024142	Cyclonite	6.72e-08	Y	-	Y
9	108-05-4	CAS-RN	DTXSID3021431	Vinyl acetate	8.3e-05	Y	-	Y
10	7803-51-2	CAS-RN	DTXSID2021157	Phosphine	-	-	-	Y
11	122-66-7	CAS-RN	DTXSID7020710	1,2-Diphenylhydrazine	1.49e-07	Y	-	Y
12	101-77-9	CAS-RN	DTXSID6022422	4,4'-Methylenedianiline	6.08e-06	Y	-	Y
13	14017-34-6	CAS-RN	DTXSID90161250	Selenium difluoride	-	-	-	-
14	75-44-5	CAS-RN	DTXSID0024260	Phosgene	-	-	-	Y
15	621-64-7	CAS-RN	DTXSID6021032	N-Nitrosodipropylamine	4.55e-07	Y	-	Y
16	75-09-2	CAS-RN	DTXSID0020868	Dichloromethane	2.02e-06	Y	-	Y
17	100-41-4	CAS-RN	DTXSID3020596	Ethylbenzene	8.32e-05	Y	-	Y
18	7440-28-0	CAS-RN	DTXSID2036035	Thallium	-	-	-	Y
19	108-88-3	CAS-RN	DTXSID7021360	Toluene	8.61e-05	Y	-	Y
20	111-44-4	CAS-RN	DTXSID9020168	Bis(2-chloroethyl) ethe	2.82e-07	Y	-	Y
21	7440-42-8	CAS-RN	DTXSID3023922	Boron	-	-	-	Y
22	7440-29-1	CAS-RN	DTXSID6049800	Thorium	-	-	-	Y

- Families of chemicals of interest
 - Polychlorinated biphenyls (PCBs)
 - Polybrominated diphenyl ethers (PBDEs)
 - Polyaromatic hydrocarbons (PAHs)

Searching Families of chemicals

Polyaromatic Hydrocarbons

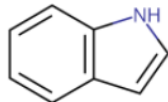
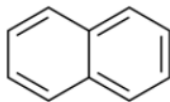
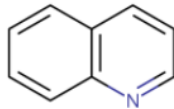
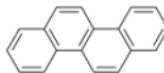
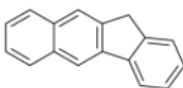
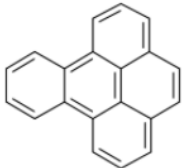
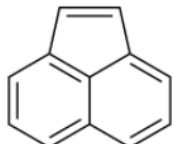
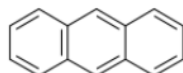
 United States Environmental Protection Agency

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Chemistry Dashboard

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<p>Representative Component</p>  <p>Indole 120-72-9</p>	<p>Representative Component</p>  <p>Naphthalene 91-20-3</p>	<p>Representative Component</p>  <p>Quinoline 91-22-5</p>	<p>Representative Component</p>  <p>Chrysene 218-01-9</p>
<p>Representative Component</p>  <p>2,3-Benzofluorene 243-17-4</p>	<p>Representative Component</p>  <p>Benzo(e)pyrene 192-97-2</p>	<p>Representative Component</p>  <p>Acenaphthylene 208-96-8</p>	<p>Representative Component</p>  <p>Anthracene 120-12-7</p>
<p>Representative Component</p>	<p>Representative Component</p>	<p>Representative Component</p>	<p>Representative Component</p>

- Specific subsets of chemicals, “lists”, can be displayed on the dashboard
- If there are chemicals that map together then these link to existing:
 - Property data
 - Hazard data
 - Exposure data
 - *In vitro* bioassay data
 - Documents and Literature

A List of Lists of Chemicals

https://comptox.epa.gov/dashboard/chemical_lists



Home

Advanced Search

Batch Search

Lists

Predictions

Downloads

Search All Data



Chemistry Dashboard

Aa ▾

Aa

Aa ▲

Select List



List Name	Number of Chemicals	List Description
40CFR355	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
Algal Toxins	54	A set of algal toxins of interest
Androgen Receptor Chemicals	110	The list of chemicals used to identify references with in vitro AR binding . From Kleinstrauer et al http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347
ATSDR Toxic Substances Portal Chemical List	200	The Agency for Toxic Substances and Disease Registry (ATSDR) is a federal public health agency of the U.S. Department of Health and Human Services.
Bisphenol Compounds	52	This list represents a collection of Bisphenol Compounds
California Office of Environmental Health Hazard Assessment	972	The OEHHA Chemical Database is a compilation of health hazard information including reference exposure levels, California public health goals, child-specific reference doses, Propos. 65 safe harbor numbers, soil-screening levels, and fish advisories
Chemicals with interesting names	17	This is a list of chemicals with interesting and fun names
EPA Integrated Risk Information System (IRIS)	510	EPA's IRIS Program identifies and characterizes the health hazards of chemicals found in the environment. Each IRIS assessment can cover a chemical, a group of related chemicals, or a complex mixture.
EPAHFR - EPA Chemicals associated with hydraulic fracturing	1640	EPAHFR lists chemicals associated with hydraulic fracturing from 2005-20013, as reported in EPA's Hydraulic Fracturing Drinking Water Assessment Final Report (Dec 2016)
EU Cosmetic Ingredients Inventory (Combined 2000/2006)	2878	EUCOSMETICS contains the Combined Inventory of Ingredients Employed in Cosmetic Products (2000, SCCNFP/0389/00 Final) and Revised Inventory (2006, Decision 2006/257/EC), prepared for NORMAN by P. von der Ohe (UBA) and R. Aalizadeh (Uni. Athens).
EU Toxrisk Dataset	230	Compounds of interest to the EU-ToxRisk Case Studies.
French Monitoring List	1171	FRENCHLIST contains substances for prospective monitoring activities in France, developed in cooperation with the NORMAN Network Working Group 1 on Prioritization. Provided by Valeria Dulio, INERIS, France. Further details on the website.

The EPA List of Hydraulic Fracturing Chemicals

EPAHFR - EPA Chemicals associated with hydraulic fracturing

Search EPAHFR Chemicals

List Details

Description: Chemicals used in hydraulic fracturing fluids and/or identified in produced water from 2005-2013, corresponding to chemicals listed in Appendix H of EPA's Hydraulic Fracturing Drinking Water Assessment Final Report (Dec 2016). Citation: U.S. EPA, Hydraulic Fracturing for Oil and Gas: Impacts from the Hydraulic Fracturing Water Cycle on Drinking Water Resources in the United States (Final Report). U.S. Environmental Protection Agency, Washington, D.C. EPA/600/R-16/236F, 2016. <https://www.epa.gov/hfstudy>

*Note that Appendix H chemical listings in Tables H-2 and H-4 were mapped to current DSSTox content, which has undergone additional curation since the publication of the original EPA HF Report (Dec 2016). In the few cases where a Chemical Name and CASRN from the original report map to distinct substances (as of Jan 2018), both were included in the current EPAHFR chemical listing for completeness; additionally, 34 previously unmapped chemicals in Table H-5 are now registered in DSSTox (all but 2 assigned CASRN) and, thus, have been added to the current EPAHFR listing.

Number of Chemicals: 1640

Download / Send

Sort by:

DTXSID



1640 chemicals

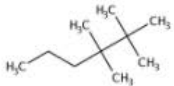
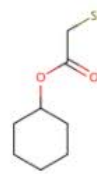
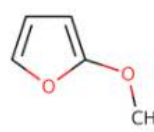
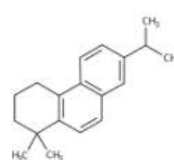
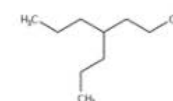

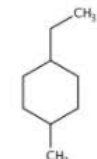

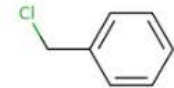
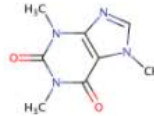
Hide:

Select all

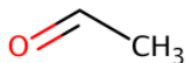


The List as "Structures"

Download / Send Sort by: DTXSID 1640 chemicals Hide: Select all

 <p>2,2,3,3-Tetramethylhexane 13475-51-5</p>	 <p>Cyclohexyl mercaptoacetate 16849-98-2</p>	 <p>2-Methoxyfuran 25414-22-8</p>	 <p>Simonellite 27530-79-8</p>	 <p>4-Propylheptane 3178-29-8</p>
 <p>7-Tetradecyne 35216-11-8</p>	 <p>1-Ethyl-4-methylcyclohexane 3728-56-1</p>	 <p>Ammonium chloride 12125-02-9</p>	 <p>Benzyl chloride 100-44-7</p>	 <p>Caffeine 58-08-2</p>

Many Hydraulic Fracturing Chemicals are “Complex”



Acetaldehyde
75-07-0

0 related chemical structures with this substance

Amines, dicoco alkyl
61789-76-2

0 related chemical structures with this substance

Amines, coco alkyldimethyl
61788-93-0

1 related chemical structure with this substance

Cristobalite
14464-46-1



Copper(I) iodide
7681-65-4

0 related chemical structures with this substance

Alcohols, C12-13, ethoxylated
66455-14-9

1 related chemical structure with this substance

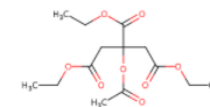
Alcohols, C12-15, ethoxylated
68131-39-5

0 related chemical structures with this substance

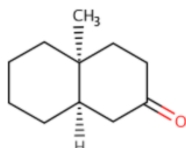
Alcohols, C14-15, ethoxylated
68951-67-7



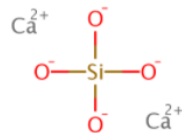
Iron
7439-89-6



Acetyltriethyl citrate
77-89-4



(4aS,8aR)-4a-Methyloctahydronaphthalen-8(1H)-one
938-06-7



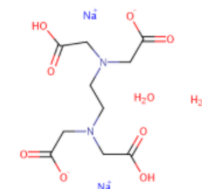
Dicalcium silicate
10034-77-2

0 related chemical structures with this substance

Diethylenetriamine reaction product with...
68647-57-4

2 related chemical structures with this substance

Di-sec-butylphenol
31291-60-8

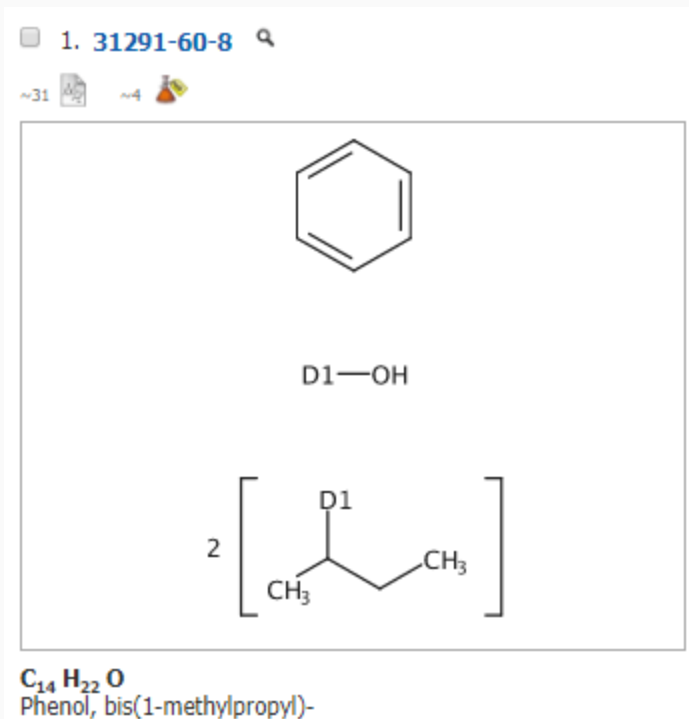


Disodium ethylenediaminetetraacetate ...
63811-92-6

- UVCBs are chemical substances of unknown or variable composition, complex reaction products and biological materials
 - Surfactants (C11-14 linear alkyl sulfonates)
 - Reaction mass of p-t-butylphenyldiphenyl phosphate and bis(p-t-butylphenyl)phenyl phosphate and triphenyl phosphate
 - Almond Oil

Di-sec-butylphenol

CAS Representation



Dashboard Representation

Di-sec-butylphenol

31291-60-8 | DTXSID5049574

Searched by DSSTox_Substance_Id: Found 1 result for 'DTXSID5049574'.

Presence in Lists

Record Information

Quality Control Notes

Related Substances

Synonyms

Links

Bioassays

Exposure

Hazard

Comments

Chemical Properties

Literature

Download / Send

Sort by: Relationship

↑

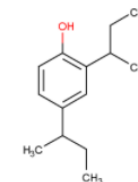
3 chemicals

Searched Chemical

2 related chemical
structures with this
substance

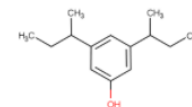
Di-sec-butylphenol
31291-60-8

Representative Isomer



2,4-Di-sec-butylphenol
1849-18-9

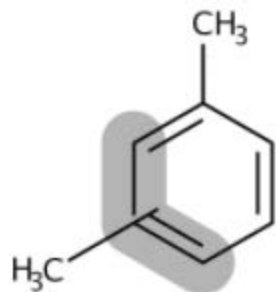
Representative Isomer



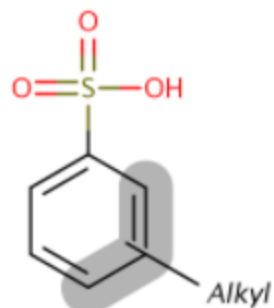
3,5-Bis(1-methylpropyl)phenol
14556-13-9

“Markush Structures”

https://en.wikipedia.org/wiki/Markush_structure



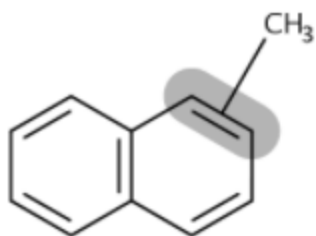
Xylenes
1330-20-7



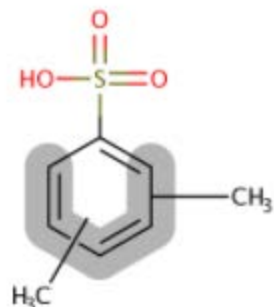
(C10-C16) Alkylbenzenesulfonic acid
68584-22-5



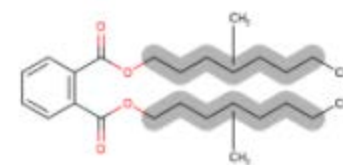
n-Nonylphenol
25154-52-3



Methylnaphthalene
1321-94-4



Sodium xylenesulfonate
1300-72-7



Diisononyl phthalate
28553-12-0

Enumeration of Markush

- Markush structures can be enumerated into chemical families

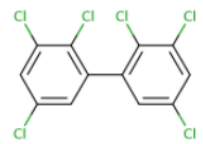
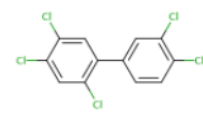
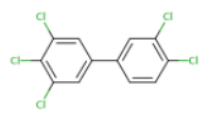
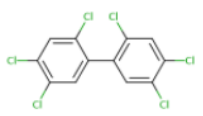
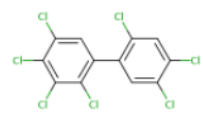
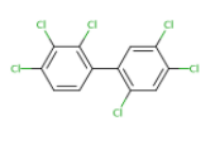
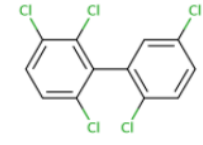
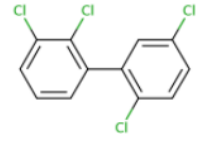
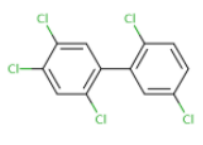
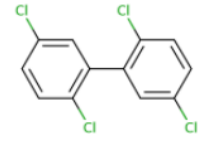
EPA United States Environmental Protection Agency

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<p>Markush Child</p>  <p>2,2',3,3',5,5'-Hexachlorobiphenyl 35694-04-3</p>	<p>Markush Child</p>  <p>2,3',4,4',5-Pentachlorobiphenyl 31508-00-6</p>	<p>Markush Child</p>  <p>3,3',4,4',5-Pentachlorobiphenyl 57465-28-8</p>	<p>Markush Child</p>  <p>2,2',4,4',5,5'-Hexachlorobiphenyl 35065-27-1</p>	<p>Markush Child</p>  <p>2,2',3,4,4',5,5'-Heptachlorobiphenyl 35065-29-3</p>
<p>Markush Child</p>  <p>2,2',3,4,4',5'-Hexachlorobiphenyl 35065-28-2</p>	<p>Markush Child</p>  <p>2,2',3,5',6-Pentachlorobiphenyl 38379-99-6</p>	<p>Markush Child</p>  <p>2,2',3,5'-tetrachlorobiphenyl 41464-39-5</p>	<p>Markush Child</p>  <p>2,2,4,5,5'-Pentochlorobiphenyl 37680-73-2</p>	<p>Markush Child</p>  <p>2,2',5,5'-Tetrachlorobiphenyl 35693-99-3</p>
<p>Markush Child</p>	<p>Markush Child</p>	<p>Markush Child</p>	<p>Markush Child</p>	<p>Markush Child</p>

Real Time Predictions

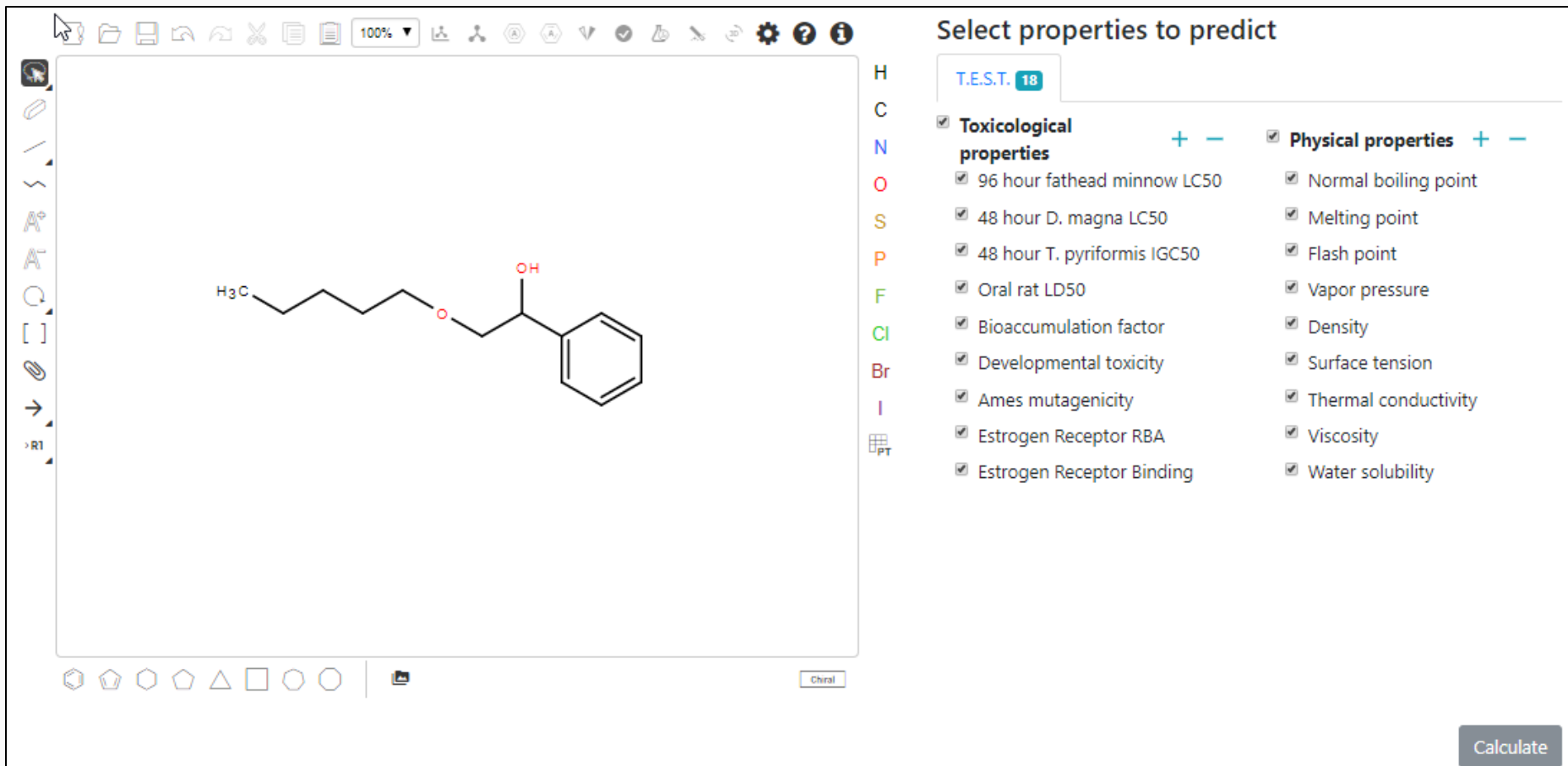
10 Years of EPA T.E.S.T Models



The screenshot shows the EPA website header with the EPA logo and navigation links: Environmental Topics, Laws & Regulations, and About EPA. A search bar is visible on the right. Below the navigation is a 'Related Topics' section with a link to 'Safer Chemicals Research'. On the right side of the header, there are links for 'CONTACT US' and 'SHARE' with social media icons for Facebook, Twitter, Pinterest, and Email. The main content area features the title 'Toxicity Estimation Software Tool (TEST)' and a section titled 'On this page:' with two links: 'QSAR Methodologies' and 'What's New in Version 4.2.1?'.

- Over 10 years of QSAR modeling at the desktop – installable Java module (from National Risk Management Research Laboratory)
- Now 750,000 chemicals predicted and real time predictions are available

Real-Time Predictions



Select properties to predict

T.E.S.T. 18

<input checked="" type="checkbox"/> Toxicological properties + -	<input checked="" type="checkbox"/> Physical properties + -
<input checked="" type="checkbox"/> 96 hour fathead minnow LC50	<input checked="" type="checkbox"/> Normal boiling point
<input checked="" type="checkbox"/> 48 hour D. magna LC50	<input checked="" type="checkbox"/> Melting point
<input checked="" type="checkbox"/> 48 hour T. pyriformis IGC50	<input checked="" type="checkbox"/> Flash point
<input checked="" type="checkbox"/> Oral rat LD50	<input checked="" type="checkbox"/> Vapor pressure
<input checked="" type="checkbox"/> Bioaccumulation factor	<input checked="" type="checkbox"/> Density
<input checked="" type="checkbox"/> Developmental toxicity	<input checked="" type="checkbox"/> Surface tension
<input checked="" type="checkbox"/> Ames mutagenicity	<input checked="" type="checkbox"/> Thermal conductivity
<input checked="" type="checkbox"/> Estrogen Receptor RBA	<input checked="" type="checkbox"/> Viscosity
<input checked="" type="checkbox"/> Estrogen Receptor Binding	<input checked="" type="checkbox"/> Water solubility

Calculate

Real-Time Predictions

Property	Experimental Value	Prediction				
		Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		4.477 -Log10(mol/L) 6.954 mg/L	4.195 -Log10(mol/L) 13.288 mg/L	3.994 -Log10(mol/L) 21.110 mg/L	3.478 -Log10(mol/L) 69.224 mg/L	6.238 -Log10(mol/L) 0.120 mg/L
48 hour D. magna LC50		4.398 -Log10(mol/L) 8.328 mg/L	3.877 -Log10(mol/L) 27.677 mg/L	4.039 -Log10(mol/L) 19.026 mg/L	4.084 -Log10(mol/L) 17.173 mg/L	5.593 -Log10(mol/L) 0.532 mg/L
48 hour T. pyriformis IGC50		4.063 -Log10(mol/L) 18.039 mg/L	3.731 -Log10(mol/L) 38.668 mg/L		3.386 -Log10(mol/L) 85.610 mg/L	5.070 -Log10(mol/L) 1.773 mg/L
Oral rat LD50		1.758 -Log10(mol/kg) 3640.950 mg/kg	1.982 -Log10(mol/kg) 2172.756 mg/kg			1.533 -Log10(mol/kg) 6101.245 mg/kg
Bioaccumulation factor		1.797 Log10 62.700	2.202 Log10 159.310	1.287 Log10 19.346	1.181 Log10 15.157	2.520 Log10 330.834
Developmental toxicity		false	false	false		true
Ames mutagenicity		false	false			false
Estrogen Receptor RBA		-3.075 Log10 8.418*10 ⁻⁴	-3.078 Log10 8.356*10 ⁻⁴	-3.720 Log10 1.907*10 ⁻⁴		-2.427 Log10 0.004
Estrogen Receptor Binding		true	true	true	false	true

- Present work in development
 - Real time OPERA predictions – TEST predictions done

- Present work in development
 - Real time OPERA prediction
 - Structure/substructure/similarity search

Prototype Development

AADashboard

atrazine Search

100%

Select properties to predict

H T.E.S.T. 18 OPERA Search

C

N Exact

O Substructure

Search result 2540 Show Isotopically Labeled Charged Salts or Mixtures Sort Similarity

 1	 0.62	 0.57	 0.57	 0.57	 0.53	 0.53	 0.53	 0.5	 0.5	 0.5
 0.5	 0.5	 0.5	 0.47	 0.44	 0.44	 0.44	 0.42	 0.42	 0.42	 0.42
 0.42	 0.42	 0.42	 0.42	 0.42	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4
 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4
 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38

Search result 2540 Show Isotopically Labeled

- Present work in development
 - Real time OPERA prediction
 - Structure/substructure/similarity search
 - Merging in other NCCT dashboard capabilities

Chemistry Dashboard

Downloads

[DSSTox Identifier to PubChem Identifier Mapping File](#)

Posted: 11/14/2016

The DSSTox to PubChem Identifiers mapping file is in TXT format and includes the PubChem SID, PubChem CID and DSSTox substance identifier (DTXSID).

SID	CID	DTXSID
316388891	20404	DTXSID30873143
316388890	10142816	DTXSID70873142
316388889	50742127	DTXSID40873139
316388888	19073841	DTXSID20873137
316388887	11505215	DTXSID00873135
316388886	25021861	DTXSID80873133
316388885	2784427	DTXSID60873131
316388884	6731	DTXSID00873130

[DSSTox identifiers mapped to CAS Numbers and Names File](#)

Posted: 11/14/2016

The DSSTox Identifiers file is in Excel format and includes the CAS Number, DSSTox substance identifier (DTXSID) and the Preferred Name.

1	casm	dsstox_substance_id	preferred_name
2	26148-68-5	DTXSID7020001	A-alpha-C
3	107-29-9	DTXSID2020004	Acetaldehyde oxime
4	60-35-5	DTXSID7020005	Acetamide
5	103-90-2	DTXSID2020006	Acetaminophen
6	968-81-0	DTXSID7020007	Acetohexamide
7	18523-69-8	DTXSID2020008	Acetone[4-(5-nitro-2-furyl)-2-thiazolyl] hydrazone
8	75-05-8	DTXSID7020009	Acetonitrile
9	127-06-0	DTXSID6020010	Acetoxime
10	65734-38-5	DTXSID6020012	N'-Acetyl-4-(hydroxymethyl) phenylhydrazine

- The CompTox Chemistry Dashboard provides access to data for ~760,000 chemicals
- An expanding list of data types and sources has been integrated
- The chemical lists of interest grows with each release
- Real time prediction models rollout has started

- Exciting array of additional searches in development

April 1st is the 2nd birthday



- The NCCT CompTox Chemistry Dashboard Development Team
- The NCCT Team of Scientists
- NERL scientists - Mass Spectrometry
- Kamel Mansouri – OPERA models
- Todd Martin – TEST predictions

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