

EPA Comptox Chemistry Dashboard: Web-based data integration hub for environmental chemistry and toxicology data

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Office of Research and Development



ISES 2017

17th October 2017

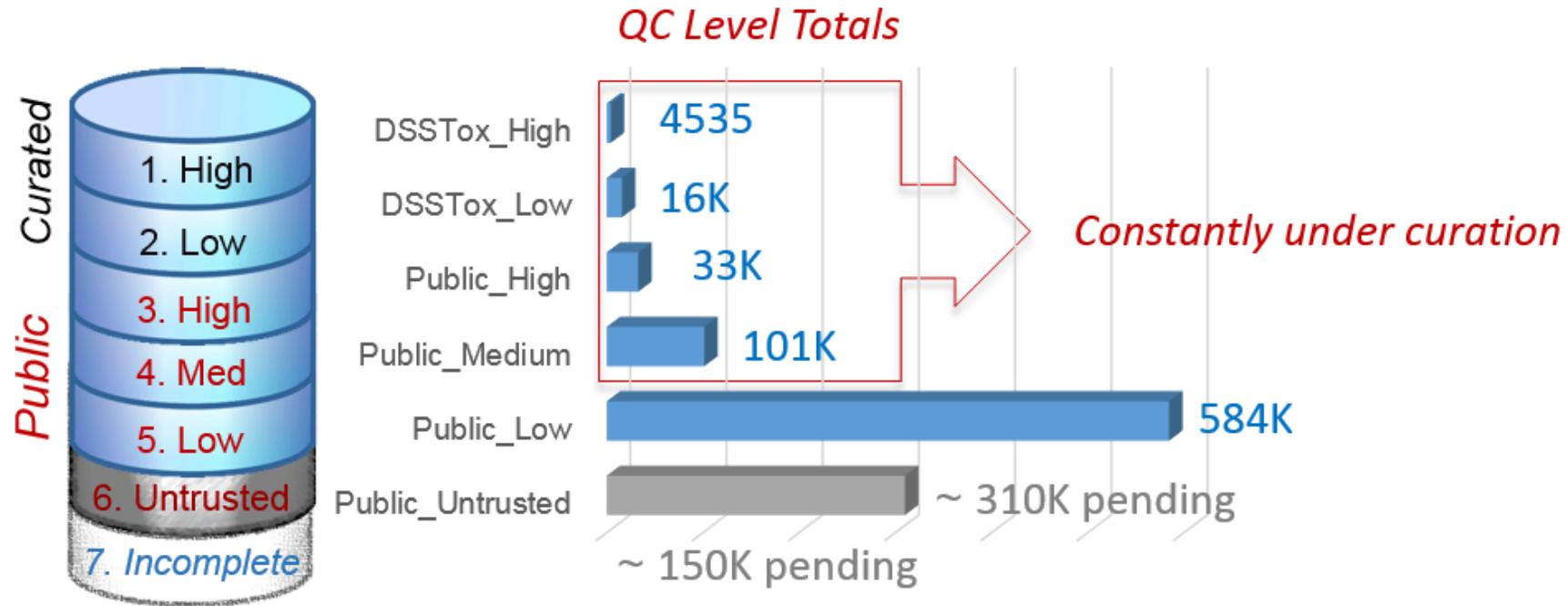
PRIMARY GOALS

- Deliver a web-based application serving up chemistry related data
- Provide public access to the results of over a decade of curation work
- Provide access to the results of our QSAR modeling work
- Transparency regarding our data and algorithms - Open Data mentality
- Deliver a central hub to link together websites of interest
- All data to be available as Open Data for download/reuse

SECONDARY GOAL

- **Develop a new cheminformatics architecture for all NCCT tools and data**

15 Years of Curating Chemistry Content



QC Levels	
DSSTox_High:	Hand curated and validated
DSSTox_Low:	Hand curated and confirmed using multiple public sources
Public_High:	Extracted from EPA SRS and confirmed to have no conflicts in ChemID and PubChem
Public_Medium:	Extracted from ChemID and confirmed to have no conflicts in PubChem
Public_Low:	Extracted from ACToR or PubChem
Public_Untrusted:	Postulated, but found to have conflicts in public sources



Comptox Chemistry Dashboard

<https://comptox.epa.gov>

The screenshot shows the Comptox Chemistry Dashboard interface. At the top is the EPA logo and navigation links: Home, Advanced Search, Batch Search, and Lists. Below this is a header with 'Chemistry Dashboard' and accessibility options. The main content area features the EPA seal, the title 'Chemistry Dashboard', and a search bar highlighted with a red box. The search bar contains the text 'Search a chemical by systematic name, synonym, CAS number, or InChIKey'. Below the search bar are options for 'Single component search' and 'Ignore isotopes'. Further down, there are links to 'See what people are saying, read the dashboard comments!' and 'Need more? Use advanced search.'. At the bottom of the main content, it displays '758 Thousand Chemicals'. The footer contains links for 'About', 'Contact', 'Privacy', 'ACToR', 'DSSTox', 'Accessibility', 'Help', and 'Downloads'.

~760,000 chemicals
>15 years of data

Search a chemical by systematic name, synonym, CAS number, or InChIKey

Single component search Ignore isotopes

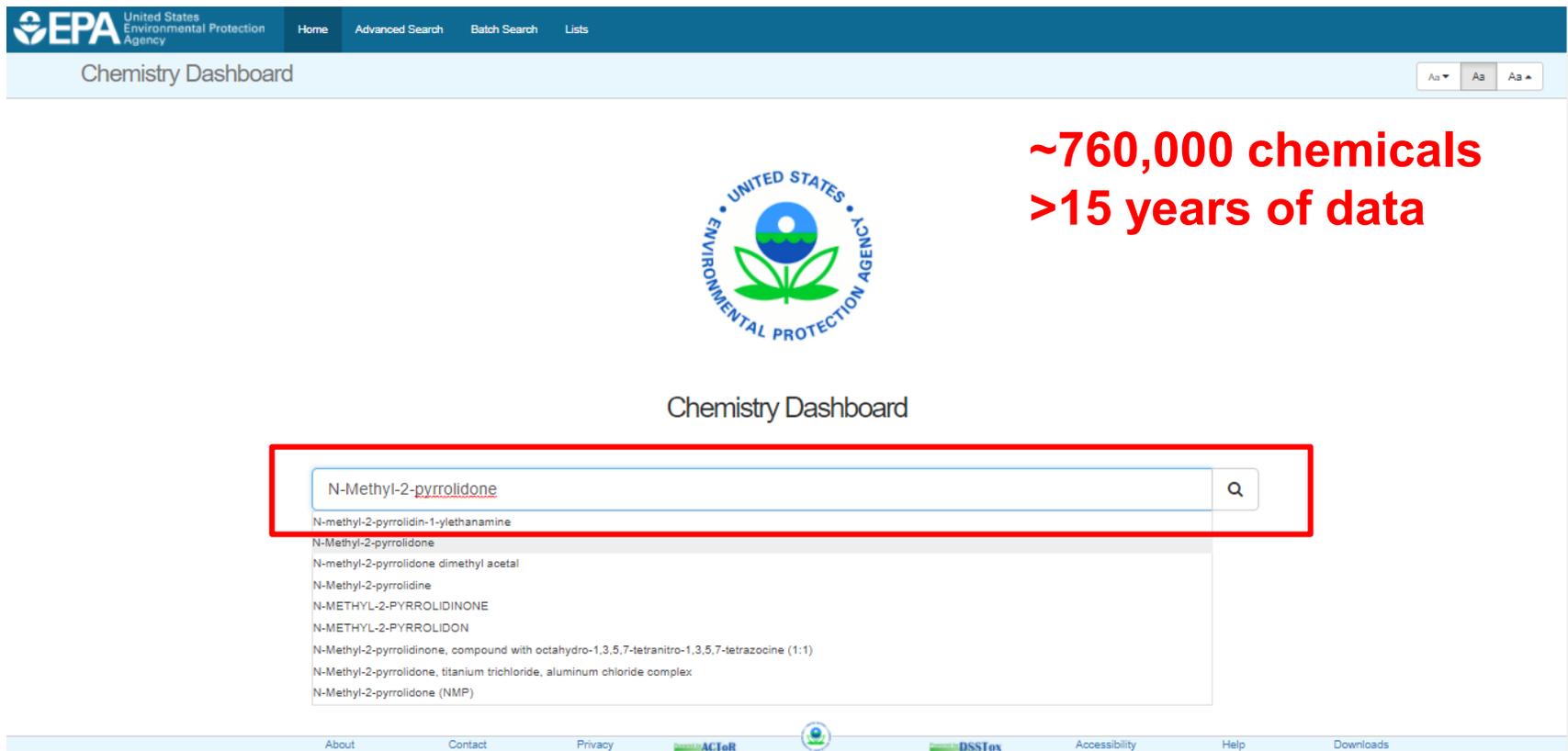
See what people are saying, read the dashboard comments!

Need more? Use advanced search.

758 Thousand Chemicals

Comptox Chemistry Dashboard

<https://comptox.epa.gov>



Chemistry Dashboard

~760,000 chemicals
>15 years of data

Chemistry Dashboard

N-Methyl-2-pyrrolidone

- N-methyl-2-pyrrolidin-1-ylethanamine
- N-Methyl-2-pyrrolidone
- N-methyl-2-pyrrolidone dimethyl acetal
- N-Methyl-2-pyrrolidine
- N-METHYL-2-PYRROLIDINONE
- N-METHYL-2-PYRROLIDON
- N-Methyl-2-pyrrolidinone, compound with octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (1:1)
- N-Methyl-2-pyrrolidone, titanium trichloride, aluminum chloride complex
- N-Methyl-2-pyrrolidone (NMP)

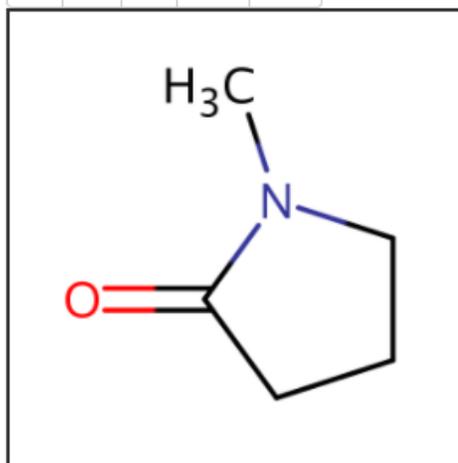
About Contact Privacy ACToR DSSTox Accessibility Help Downloads

Chemical Page

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856

© Searched by Synonym from Valid Source: Found 1 result for 'N-METHYLPYRROLIDONE'.



Wikipedia

Intrinsic Properties

Molecular Formula: C₅H₉NO



Average Mass: 99.133 g/mol



Monoisotopic Mass: 99.068414 g/mol



Structural Identifiers

Related Compounds

Presence in Lists

Record Information

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

External Links

Chemical Properties

Summary

Download as:

TSV

Excel

SDF

LogP: Octanol-Water

Water Solubility

Density

Flash Point

Melting Point

Boiling Point

Surface Tension

Thermal Conductivity

Vapor Pressure

Viscosity

LogKoa: Octanol-Air

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	-0.380 (1)	-0.329 (5)	-0.380	-0.329	-0.380	-0.494 to -0.110	-
Water Solubility	10.1 (1)	6.68 (4)	10.1	6.68	10.1	1.48 to 12.8	mol/L
Density	-	1.02 (2)	-	1.02	-	1.01 to 1.03	g/cm ³
Flash Point	-	75.7 (2)	-	75.7	-	65.2 to 86.1	°C
Melting Point	-23.8 (8)	1.32e-01 (4)	-24.0	1.32e-01	-24.0 to -23.0	-10.2 to 25.9	°C
Boiling Point	203 (6)	199 (5)	204	199	202 to 204	191 to 202	°C
Surface Tension	-	33.8 (1)	-	33.8	-	-	dyn/cm
Thermal Conductivity	-	158 (1)	-	158	-	-	mW/(m ² K)
Vapor Pressure	3.45e-01 (1)	5.21e-01 (4)	3.45e-01	5.21e-01	3.45e-01	1.71e-01 to 9.99e-01	mmHg
Viscosity	-	3.61 (1)	-	3.61	-	-	cP
LogKoa: Octanol-Air	-	3.84 (1)	-	3.84	-	-	-
Henry's Law	3.20e-09 (1)	9.15e-09 (1)	3.20e-09	9.15e-09	-	-	atm-m ³ /mole
Index of Refraction	-	1.47 (1)	-	1.47	-	-	-

Chemical Properties

Env. Fate/Transport

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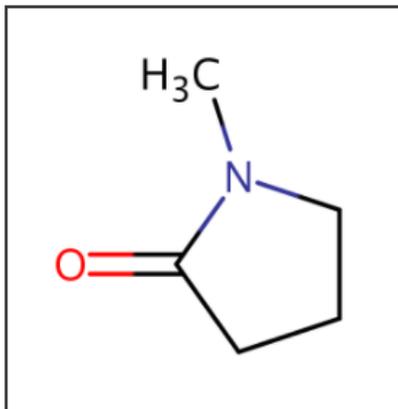
Multiple Prediction Algorithms

Experimental		
Source	Result	
PhysPropNCCT	-0.380	

Predicted		
Source	Result	Calculation Details
EPISUITE	-0.110	Not Available
NICEATM	-0.494	Not Available
ACD/Labs Consensus	-0.345	Not Available
ACD/Labs	-0.398	Not Available
OPERA	-0.300	OPERA Model Report

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856



Model Results

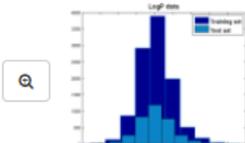
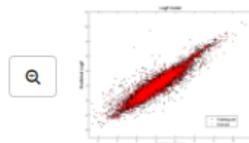
Predicted value: -0.300

Global applicability domain: **Inside** ⓘ

Local applicability domain index: 0.88 ⓘ

Confidence level: 0.81 ⓘ

Model Performance



Weighted KNN model

QMRF

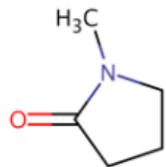
5-fold CV (75%)

Training (75%)

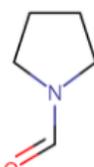
Test (25%)

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.88	0.67	0.88	0.78

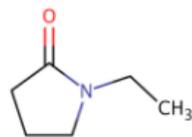
Nearest Neighbors from the Training Set



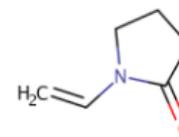
N-Methyl-2-pyrrolidone
Measured: -0.380
Predicted: -0.300



Proinal
Measured: -0.320
Predicted: -0.226



1-Ethyl-2-pyrrolidinone
Measured: -0.0400
Predicted: -0.211



N-Vinyl-2-pyrrolidone
Measured: 0.37
Predicted: 2.65e-01

LogP (00000002).pdf - Adobe Acrobat Pro

File Edit View Window Help

Create [Icons] 1 / 11 125% Tools Fill & Sign Comment

Bookmarks

- 1.QSAR identifier
 - 1.1.QSAR identifier (title)
 - 1.2.Other related models
 - 1.3.Software coding the model
- 2.General information
 - 2.1.Date of QMRF
 - 2.2.QMRF author(s) and contact details
 - 2.3.Date of QMRF update(s)
 - 2.4.QMRF update(s)
 - 2.5.Model developer(s) and contact details
 - 2.6.Date of model development and/or publication
 - 2.7.Reference(s) to main scientific papers and/or software package
 - 2.8.Availability of information about the model
 - 2.9.Availability of another QMRF for exactly the same model
- 3.Defining the endpoint - OECD Principle 1
 - 3.1.Species
 - 3.2.Endpoint
 - 3.3.Comment on endpoint
 - 3.4.Endpoint units
 - 3.5.Dependent variable
 - 3.6.Experimental protocol
 - 3.7.Endpoint data quality and variability
- 4.Defining the algorithm - OECD Principle 2
 - 4.1.Type of model
 - 4.2.Explicit algorithm
 - 4.3.Descriptors in the model
 - 4.4.Descriptor selection
 - 4.5.Algorithm and descriptor generation
 - 4.6.Software name and version for descriptor generation
 - 4.7.Chemicals/Descriptors ratio
- 5.Defining the applicability domain - OECD Principle 3
 - 5.1.Description of the applicability domain of the model

	<p>QMRF identifier (JRC Inventory): To be entered by JRC</p> <p>QMRF Title: LogP: Octanol-water partition coefficient prediction from the NCCT Models Suite.</p> <p>Printing Date: Apr 25, 2016</p>
-------------------------------------------------------------------------------------	--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

1.QSAR identifier

1.1.QSAR identifier (title):
LogP: Octanol-water partition coefficient prediction from the NCCT_Models Suite.

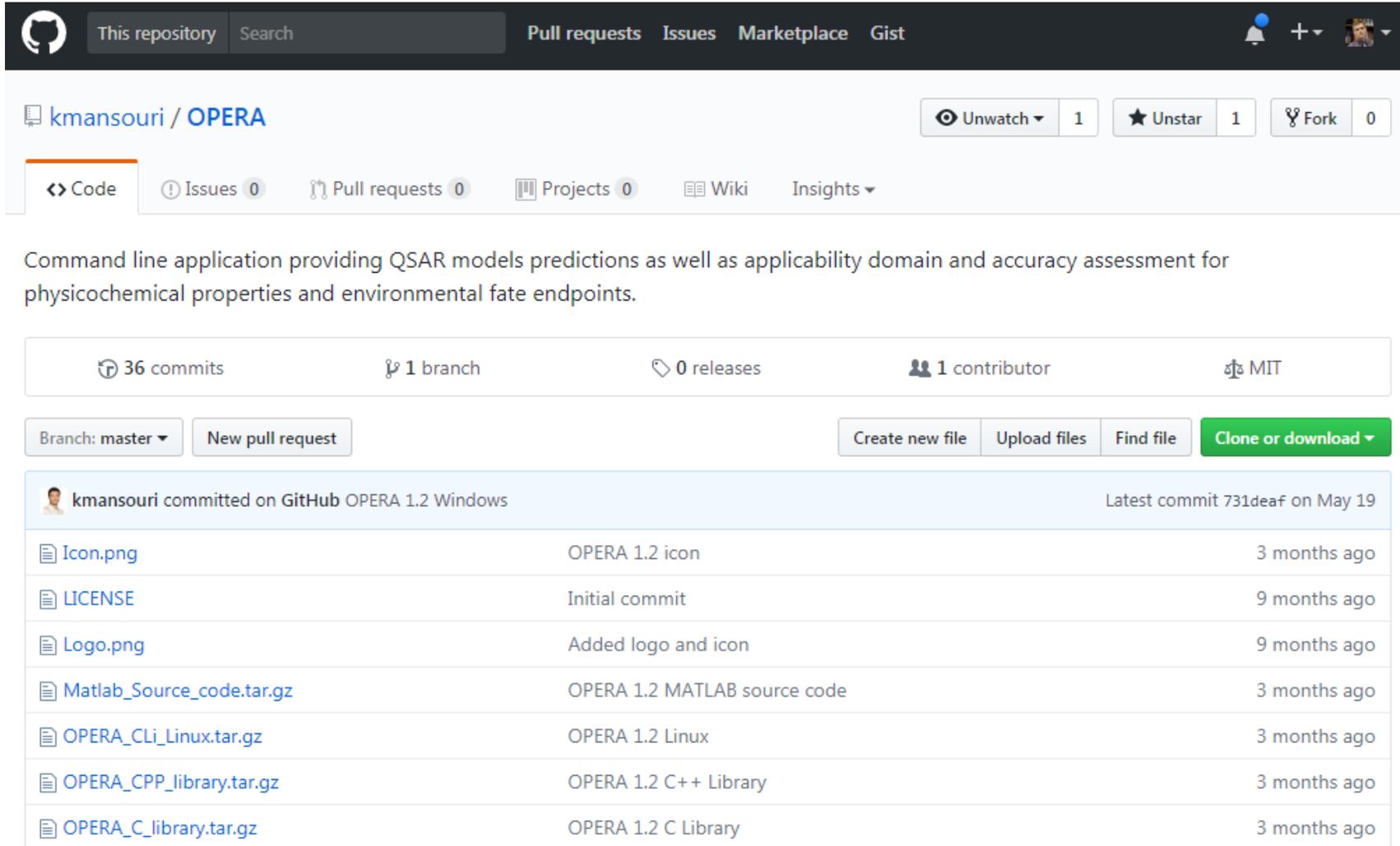
1.2.Other related models:
 No related models

1.3.Software coding the model:
 NCCT_models V1.02
 Suite of QSAR models to predict physico-chemical properties and environmental fate of organic chemicals
 Kamel Mansouri (mansouri.kamel@epa.gov; mansourikamel@gmail.com);
<https://comptox.epa.gov/dashboard/>

PaDEL descriptors V2.21
 Open source software to calculate molecular descriptors and fingerprints.
 Chun Wei Yap (phayapc@nus.edu.sg)
<http://padel.nus.edu.sg/software/padeldescriptor>

MATLAB
 MATrix LABoratory is a multi-paradigm numerical computing environment and fourth-generation

Transparency: OPERA on GitHub



The screenshot shows the GitHub repository page for `kmansouri / OPERA`. The repository is currently on the `master` branch. It has 36 commits, 1 branch, 0 releases, and 1 contributor. The license is MIT. The repository description is: "Command line application providing QSAR models predictions as well as applicability domain and accuracy assessment for physicochemical properties and environmental fate endpoints." The file list includes:

File Name	Description	Commit Time
<code>Icon.png</code>	OPERA 1.2 icon	3 months ago
<code>LICENSE</code>	Initial commit	9 months ago
<code>Logo.png</code>	Added logo and icon	9 months ago
<code>Matlab_Source_code.tar.gz</code>	OPERA 1.2 MATLAB source code	3 months ago
<code>OPERA_CLI_Linux.tar.gz</code>	OPERA 1.2 Linux	3 months ago
<code>OPERA_CPP_library.tar.gz</code>	OPERA 1.2 C++ Library	3 months ago
<code>OPERA_C_library.tar.gz</code>	OPERA 1.2 C Library	3 months ago

<https://github.com/kmansouri/OPERA.git>

Toxicity Values

Bioavailability Metric

Download as:

Exposure Limit	Type	Subtype	Value	Units	Study Type	Exposure Route	Study Duration	Species	Media	Details	Source
Point Of Departure	TD50	-	20.7	mM/kg-day	-	-	-	-	-	DSSTox C...	ACToR
Regulatory Toxicity Value	TD50	-	2050	mg/kg-day	-	-	-	-	-	DSSTox C...	ACToR
Effect Level	LEL	systemic	619	mg/kg-day	subchronic	oral	subchronic	mouse	-	Study ID: ...	ToxRefDB
Misc Hazard Information	NEL	systemic	277	mg/kg-day	subchronic	oral	subchronic	mouse	-	Study ID: ...	ToxRefDB
Screening Level	LEL	systemic	25.0	mg/kg-day	subchronic	oral	subchronic	dog	-	Study ID: ...	ToxRefDB
Uncertainty Factor	NEL	systemic	25.0	mg/kg-day	subchronic	oral	subchronic	dog	-	Study ID: ...	ToxRefDB
	LEL	systemic	173	mg/kg-day	chronic	oral	chronic	mouse	-	Study ID: ...	ToxRefDB
	NEL	systemic	115	mg/kg-day	chronic	oral	chronic	mouse	-	Study ID: ...	ToxRefDB
	LEL	systemic	678	mg/kg-day	chronic	oral	chronic	rat	-	Study ID: ...	ToxRefDB
	NEL	systemic	283	mg/kg-day	chronic	oral	chronic	rat	-	Study ID: ...	ToxRefDB
	LEL	systemic	1230	mg/kg-day	subacute	oral	subacute	rat	-	Study ID: ...	ToxRefDB
	NEL	systemic	493	mg/kg-day	subacute	oral	subacute	rat	-	Study ID: ...	ToxRefDB
	LEL	systemic	2130	mg/kg-day	subacute	oral	subacute	mouse	-	Study ID: ...	ToxRefDB
	NEL	systemic	920	mg/kg-day	subacute	oral	subacute	mouse	-	Study ID: ...	ToxRefDB

Product Composition Details

Chemical Weight Fractions ⓘ

Download as: TSV Excel

<u>Product Name</u>	<u>Product Use Category</u>	<u>Minimum Weight Fraction</u>	<u>Maximum Weight Fraction</u>	<u>Data Type</u>	<u>Source</u>
citristrip canadian stripping...	home maintenance: stripper	0.65	0.7	MSDS	Retail Product Categories/...
citristrip stripping gel qog7...	home maintenance: stripper	0.4	0.55	MSDS	Retail Product Categories/...
gumout 2 part professional...	auto products: auto fluids a...	0.3	0.4	MSDS	Retail Product Categories/...
minwax water based wipe ...	home maintenance: finish	0.06	0.06	MSDS	Retail Product Categories/...
10-02199- calico tip & glue...	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
artificial nail remover 728 1	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
calico tip & glue remover 1	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
kiss nail remover 1	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
waterborne clear wood fini...	home maintenance: finish	0.01	0.05	MSDS	Retail Product Categories/...

In vitro Bioassay Data

- **In vitro bioassays** are used to determine the biological activity of a substance – **ToxCast and Tox21 projects**
- A decade of measurements, and millions of dollars of data integrated into the dashboard

Download as: Show:

Assay Name	Hit Call ↑	Top	Scaled Top	AC50	log AC50	Intended Target Family
TOX21_Aromatase_Inhibition	ACTIVE	60.7	1.94	28.1	1.45	cyp
TOX21_ERa_LUC_BG1_Agonist	ACTIVE	28.9	1.14	49.8	1.70	nuclear receptor
NVS_TR_hDAT	ACTIVE	55.8	2.79	31.8	1.50	transporter
BSK_CASM3C_SAA_up	ACTIVE	0.129	1.28	0.0116	-1.93	cell adhesion molecules
ATG_RXRb_TRANS_up	ACTIVE	3.58	3.47	23.5	1.37	nuclear receptor
APR_HepG2_MitoMembPot_72h_dn	ACTIVE	0.951	1.30	0.413	-0.384	cell morphology

Names and Identifiers

Found 40 synonyms

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

 Copy all Synonyms

N-Methyl-2-pyrrolidone

1-Methylpyrrolidin-2-one

2-Pyrrolidinone, 1-methyl-

872-50-4 Active CAS-RN

2-Pyrrolidinone, 1-methyl-

1-Methyl-2-pyrrolidinone

1-Methyl-2-pyrrolidon

1-Methyl-2-pyrrolidone

1-Methyl-5-pyrrolidinone

1-Methylazacyclopentan-2-one

1-Methylpyrrolidone

1-metil-2-pirrolidona

2-Pyrrolidinone, 1-methyl-

2-Pyrrolidone, 1-methyl-

Microposit 2001

M-Pyrol

Integrated Literature Searching

PubChem

 BioAssay  Compound  Substance

Google
Scholar

atrazine

PubMed

PubMed comprises more than 26 million citations for biomedical literature from MEDLINE, life science journals, and online books. Citations may include links to full-text content from PubMed Central and publisher web sites.

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

External Links

Integrated Literature Searching

Google Scholar

PubMed Abstract S...

PubChem Articles

PubChem Patents

Select Term:

Hazard

AND

RfD OR reference dose



"RfD OR reference dose" AND "Hazard" AND "872-50-4" OR "N-Methyl-2-py



Scholar

About 22 results (0.05 sec)

Articles

[Solvent Substitution: An Analysis of Comprehensive Hazard Screening Indices](#)

M Debia, D Bégin, M Gérin - *Journal of occupational and ...*, 2011 - oeh.tandfonline.com

Case law

... Reliability and weighting factors were not used. Armenti and Moure-Eraso(22) used the same FHS index, using six **hazard** categories, to compare replacement options. ...

My library

872-50-4 N-Methyl-2-pyrrolidone 45.4 13 1.46E-03 11 4.55 6 20 4 ...

[Related articles](#) [All 4 versions](#) [Cite](#) [Save](#)

Any time

[Effects of 'inactive'ingredients on bees](#)

Since 2017

CA Mullin - *Current Opinion in Insect Science*, 2015 - Elsevier

Since 2016

... tallow amines, organosilicone ethoxylates and co-solvents such as **N-methyl-2-pyrrolidone** (NMP)

Since 2013

[7 ... of tools to environmentally monitor residues and determine their relative **hazard** to bees. ... Defining a benchmark or **reference dose**, particularly for bee viruses [51], for what can ...

Custom range...

[Cited by 9](#) [Related articles](#) [All 2 versions](#) [Web of Science: 6](#) [Cite](#) [Save](#) [More](#)

Sort by relevance

[Biological monitoring: exquisite research probes, risk assessment, and routine exposure measurement](#)

Sort by date

WM Draper - *Analytical chemistry*, 2001 - ACS Publications

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Create alert

[Evolution of chemical-specific adjustment factors \(CSAF\) based on recent international experience; increasing utility and facilitating regulatory acceptance](#)

VS Bhat, ME Meek, M Valcke, C English... - *Critical Reviews in ...*, 2017 - Taylor & Francis

... As shown in the right side of Figure 2, uncertainty is taken into consideration at all tiers of **hazard** assessment. ... For decades, developing "safe doses" such as the oral **reference dose** (RfD), the inhaled reference concentration (RfC) or the acceptable or tolerable daily intake (ADI ...

[All 3 versions](#) [Cite](#) [Save](#)

Chemical Properties

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Toxicity Values (Beta)

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Similar Molecules (Beta)

Synonyms

Literature

External Links

Integrated Literature Searching

- Google Scholar
- PubMed Abstract ...**
- PubChem Articles
- PubChem Patents

Select Term:

Select a Query Term

- Select a Query Term
- Hazard
- Fate and Transport
- Metabolism/PK/PD
- Chemical Properties
- Exposure
- Mixtures
- Male Reproduction
- Androgen Disruption
- Female Reproduction
- GeneTox
- Embryo and embryonic development
- Child (infant through adolescent)
- Dust and Exposure

ing Articles

rrolidone" OR "N-methylpyrrolidone"



Search and Count

Integrated Literature Searching

Google Scholar

PubMed Abstract Sifter

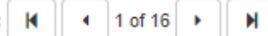
PubChem Articles

PubChem Patents

Edit the Query Before Retrieving Articles

("872-50-4" OR "N-Methyl-2-pyrrolidone" OR "N-methylpyrrolidone") AND (exposure OR near-field OR far-field OR SHEDS[tiab] AND ENVIRONMENTAL MONITORING)

1	0	0	0	0	24078144	2013	Biological monitoring and health effects of low-level exposure to N-methyl-2-pyrrolidone: a cross-sectional study.
0	0	0	0	0	23337464	2013	Biomonitoring of exposure to N-methyl-2-pyrrolidone in workers of the automobile industry.
0	0	0	0	0	19875680	2009	Quantitative risk analysis for N-methyl pyrrolidone using physiologically based pharmacokinetic and benchmark dos...
0	0	0	0	0	16897094	2006	Human volunteer study on the influence of exposure duration and dilution of dermally applied N-methyl-2-pyrrolidon...

Record:  1 of 16

Title: [Not Available].

Abstract: N-Ethyl-2-pyrrolidone (NEP), a polar aprotic solvent, is used in many applications as substitute for the structural analogue N-methyl-2-pyrrolidone (NMP), e. g. for surface coatings, in cleaning agents and paint strippers. Monitoring studies indicate that individuals within the general public, without occupational exposure, may be exposed to NEP to an extent, which is comparable to NMP. As NMP, NEP presents a potential health hazard due to its developmental toxicity and teratogenicity. Exposure to NEP can be quantified by the determination of the excretion of its urinary metabolites 5-Hydroxy-N-ethyl-2-pyrrolidone (5-HNEP) and 2-Hydroxy-N-ethylsuccinimide (2-HESI). For the derivation of HBM values, the german Human Biomonitoring Commission (HBM commission) evaluated different toxicological endpoints and finally decided on the BMDL05 and the BMD10 for the endpoint "reduced grasp intensity" of a subchronic feeding study with rats as point of departure (POD) for further procedural steps. The resulting HBM-I and HBM-II values for the sum of the metabolites 5-HNEP and 2-HESI in the urine of children are 10 resp. 25 mg/l and in the urine of adults are 15 resp. 40 mg/l. If the HBM values are exceeded, a check-up will be necessary at first. Measurements above the HBM-II value give cause for concern, especially for pregnant women. Air measurements to determine the source of exposure can be useful. The possibility of skin absorption from use of

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

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Synonyms

Literature

External Links

Pubmed Abstract Sifter

Select Term:

▶ Exposure ▼

Retrieve Articles

0 Articles

Add additional query terms to filter abstracts:

developmental

reproductive

occupational

Search and Count

Edit the Query Before Retrieving Articles

("872-50-4" OR "N-Methyl-2-pyrrolidone" OR "N-methylpyrrolidone") AND (exposure OR near-field OR far-field OR SHEDS[tiab] AND ENVIRONMENTAL MONITORING)

dev...	rep...	occ...	Total	PMID	Pu...	Title
0	0	1	1	24078144	2013	Biological monitoring and health effects of low-level exposure to N-methyl-2-pyrrolidone: a cross-sectional study.
1	0	0	1	23337464	2013	Biomonitoring of exposure to N-methyl-2-pyrrolidone in workers of the automobile industry.
0	0	2	2	19875680	2009	Quantitative risk analysis for N-methyl pyrrolidone using physiologically based pharmacokinetic and benchmark dos...
0	0	1	1	16897094	2006	Human volunteer study on the influence of exposure duration and dilution of dermally applied N-methyl-2-pyrrolidon...
0	0	0	0	16362322	2005	Ambient monitoring and biomonitoring of workers exposed to N-methyl-2-pyrrolidone in an industrial facility

Record: [◀] [◀] 1 of 16 [▶] [▶]

Title: Stillbirth after occupational exposure to N-methyl-2-pyrrolidone. A case report and review of the literature.

Abstract: N-methyl-2-pyrrolidone is a solvent that is increasingly used in a variety of industries, including petroleum refining, microelectronics, pesticide formulation, and veterinary medicine. Animal studies have demonstrated fetotoxic effects after maternal exposure to doses that have minimal to no adverse effect on the mothers. The fetotoxicity comprises resorption, stillbirth, and low birthweight and delayed ossification in surviving young. We report a human case of intrauterine growth retardation followed by fetal demise at 31 weeks gestation. The mother was a laboratory worker with no other apparent risk factors, who sustained occupational exposure to N-methyl-2-pyrrolidone throughout the first trimester of pregnancy. Laboratory work and solvent exposure have both previously been associated with adverse reproductive outcomes. Laboratories and other industries that use suspected reproductive toxins should have reproductive health policies in place that allow for decision-making based on toxicologic review, exposure assessment, and medical evaluation. These policies should allow for voluntary removal of prospective parents until environmental assessment and controls are instituted.

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

External Links

Links to Other Resources

General

 EPA Substance Re...

 NIST Chemistry W...

 Household Product...

 PubChem

 Chemspider

 CPCat

 DrugBank

 HMDB

 Wikipedia

 MSDS Lookup

 ChEMBL

 Chemical Vendors

 Consumer Product...

Toxicology

 ACToR

 DrugPortal

 CCRIS

 ChemView

 CTD

 EPA

 EPA

 GPO

 HSDB

 ToxCast Dashboar...

 LactMed

 ACToR PDF Report

 International Toxicit...

Publications

 Toxline

 Environmental Heal...

 NIEHS

 National Toxicology...

 Google Books

 EPA

 EPA

 GPO

 Federal Register

 Regulations.gov

 Springer Materials

 BioCaddie DataMed

 RSC Publications

Analytical

 National Environme...

 MONA: MassBank ...

 Tox21 Analytical Data

 RSC Analytical Abs...

 FOR-IDENT

The Office of the Federal Register (OFR) of the National Archives and Records Administration (NARA), and the U.S. Government Printing Office (GPO) jointly administer the FederalRegister.gov website.

Example External Links...

U.S. Department of Health & Human Services www.hhs.gov

Household Products Database
Health & Safety Information on Household Products

National Institutes of Health
National Library of Medicine
Specialized Information Services 

English | Español

ChemHAT.org
Chemical Hazard and Alternatives Toolbox

ABOUT CHEMHAT

ECHA
EUROPEAN CHEMICALS AGENCY

Search the ECHA Website

N-methylpyrrolidone
CAS: 872-50-4

How can this chemical affect my health?

Acute (Short Term) Health Effects

-  **Irritates the Eyes** - Can irritate or cause serious damage to the eye.

Chronic (Long Term) Health Effects

-  **Birth Defects** - Can cause developing child including defects, low birth weight, biological or behavioral abnormalities as the child grows.
-  **Other Health Effects** - Can cause serious damage on contact or ingestion.

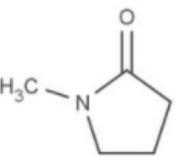
ECHA > Substance Information > 1-methyl-2-pyrrolidone

Substance information

Infocards are automatically generated based on industry data. [What is an infocard?](#)

1-methyl-2-pyrrolidone

Other names: Regulatory process names [4] Trade names [22] Other names [1] IUPAC names [27]

Substance identity	Hazard classification & labelling	Properties of concern
<p>EC / List no.: 212-828-1</p> <p>CAS no.: 872-50-4</p> <p>Mol. formula: C₅H₉NO</p> 	<p>Danger! According to the harmonised classification and labelling (ATP09) approved by the European Union, this substance may damage the unborn child, causes serious eye irritation, causes skin irritation and may cause respiratory irritation.</p> <p>Additionally, the classification provided by companies to ECHA in REACH registrations identifies that this substance may damage fertility or the unborn child.</p>	<p>R</p> <p>Important to know</p> <ul style="list-style-type: none"> Substance of very high concern (SVHC) and included in the candidate list for authorisation. <p>How to use it safely</p> <ul style="list-style-type: none"> ECHA has no data from registration dossiers on the precautionary measures for using this substance. Guidance on the safe use of the substance provided by manufacturers and importers of this substance.

About this substance

This substance is manufactured and/or imported in the European Economic Area in 10 000 - 100 000 tonnes per year.

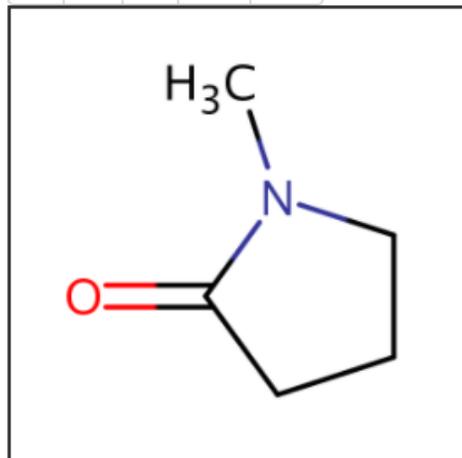
This substance is used by consumers, by professional workers (widespread uses), in formulation or re-

Managing structure relationships

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856

© Searched by Synonym from Valid Source: Found 1 result for 'N-METHYLPYRROLIDONE'.



Wikipedia

Intrinsic Properties

Structural Identifiers

Related Compounds

Same Connectivity: [3 records](#) (based on first layer of InChI)

Mixtures, Components, and Neutralized Forms: [11 records](#) (based on QSAR ready mappings and with the compound as a component of a mixture)

Similar Compounds: [970 records](#) (based on Tanimoto coefficient > 0.8)

Presence in Lists

Record Information

Managing structure relationships

Chemistry Dashboard

View Selected

Hide Isotopes

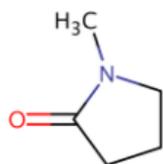
Hide Multicomponent Chemicals



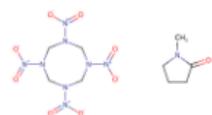
Aa ▼

Aa

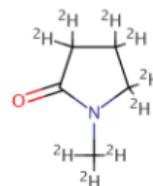
Aa ▲



N-Methyl-2-pyrrolidone
872-50-4



2-Pyrrolidinone, 1-methyl-, compd. wit...
3531-64-4



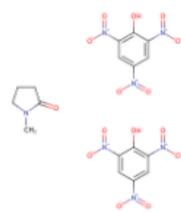
1-(²H₂²H₂)Met...
185964-60-7



HCl
1-Methylpyrrolidin-2-one--hydrogen c...
16889-93-3



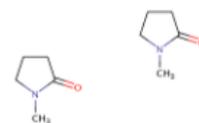

Sulfuric acid--1-methylpyrrolidin-2-on...
80997-96-2



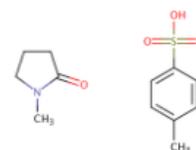
1-Methylpyrrolidin-2-one--2,4,6-trinitro...
61727-04-6




Nitric acid--1-methylpyrrolidin-2-one (...
918666-25-8




Sulfuric acid--1-methylpyrrolidin-2-on...
918666-23-6



4-Methylbenzene-1-sulfonic acid--1-m...
918659-71-9



H₂O
1-Methylpyrrolidin-2-one--water (1/2)
32997-25-4



Poly (acrylamide-co-acrylic acid), partial sodium salt

62649-23-4 | DTXSID1049722 ⓘ

ⓘ Searched by Approved Name: Found 1 result for 'Poly (acrylamide-co-acrylic acid), partial sodium salt'.

Record Information

Citation

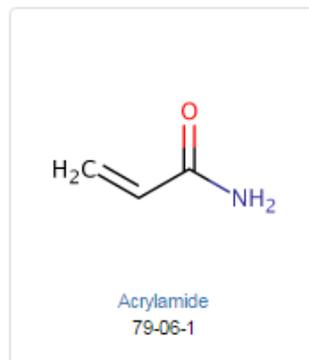
U.S. Environmental Protection Agency. Chemistry Dashboard. <https://comptox.epa.gov/dashboard/DTXSID1049722> (accessed February 12, 2017), Poly (acrylamide-co-acrylic acid), partial sodium salt

Data Quality **80%**

Manually curated and no conflicts in multiple public sources

Related Chemicals

Found 2 chemicals





UVCB Chemicals

- UVCB chemicals - Unknown or Variable Composition, Complex Reaction Products and Biological Materials
- Many different types of UVCB chemicals
 - Surfactants with undefined composition
 - Petroleum Distillates
 - Gelatins, hydrozylates
 - Formaldehyde, reaction products with diethanolamine
 - Fatty acids, linseed-oil, compds. with triethylamine

Managing UVCB Relationships

Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

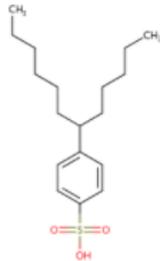
i Searched by Synonym: Found 1 result for
'Linear alkylbenzene sulfonate'.

Presence in Lists

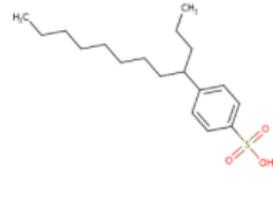
Surfactant List Screened in Swiss Wastewater (2014)

Surfactant List Screened in Swiss Wastewater (2014)

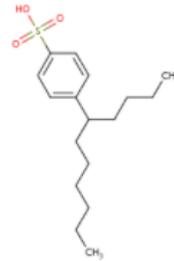
EAWAGSURF is a list of surfactants screened in Swiss wastewater effluents as part of a 2014 study. Structures/mixtures are being progressively curated and linked (Schymanski/Williams). Further details in Schymanski et al 2014, DOI: 10.1021/es4044374



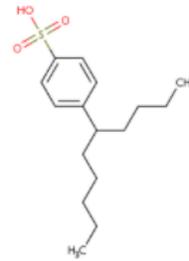
4-(Dodecan-6-yl)benzene-1-sulfon...
23003-92-1



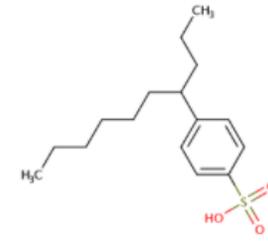
4-(dodecan-4-yl)benzene-1-sulfoni...
NOCAS_862870



C11-LAS
NOCAS_881097



4-(decan-5-yl)benzene-1-sulfonic ...
NOCAS_881146



4-(decan-4-yl)benzenesulfonic acid
NOCAS_891333

T.E.S.T services public ALPHA

- 96hr fathead minnow 50% lethal concentration (LC50)
- 48hr daphnia magna 50% lethal concentration (LC50)
- Tetrahymena pyriformis 50% growth inhibition conc. (IGC50)
- Oral rat 50% lethal dose (LD50)
- Bioconcentration Factor (BCF)
- Developmental Toxicity (DevTox)
- Ames Mutagenicity (Mutagenicity)
- Normal boiling point, Flash point, Melting point
- Surface tension, Viscosity, Water Solubility
- Thermal Conductivity, Vapor Pressure, Density

- **EXAMPLE:** [https://comptox.epa.gov/dashboard/web-test/WS?smiles=C1C\(Cl\)\(Cl\)Cl](https://comptox.epa.gov/dashboard/web-test/WS?smiles=C1C(Cl)(Cl)Cl)

Use Cases

- I have a list of chemical names and CAS Registry Numbers
- What can the dashboard tell me about?
 - What are the chemical structures???
 - Are there predicted properties available?
 - Are there high throughput screening data?
 - What toxicity data are available?
 - Can I download the data for me to use?

Real World Applications – Names to Chemicals



EPA
United States
Environmental Protection
Agency

EPA/600/R-16/364 | December 2016 | www.epa.gov

ATSDR
AGENCY FOR TOXIC SUBSTANCES
AND DISEASE REGISTRY

COMMUNITY PRODUCT SAFETY CONSUMER ACTION

HEALTH AND HUMAN SERVICES

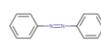
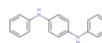
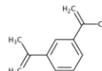
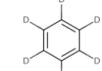
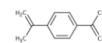
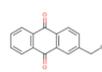
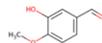
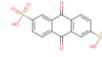
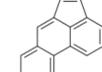
CDC
CENTERS FOR DISEASE
CONTROL AND PREVENTION

Federal Research Action Plan on Recycled Tire Crumb Used on Playing Fields and Playgrounds

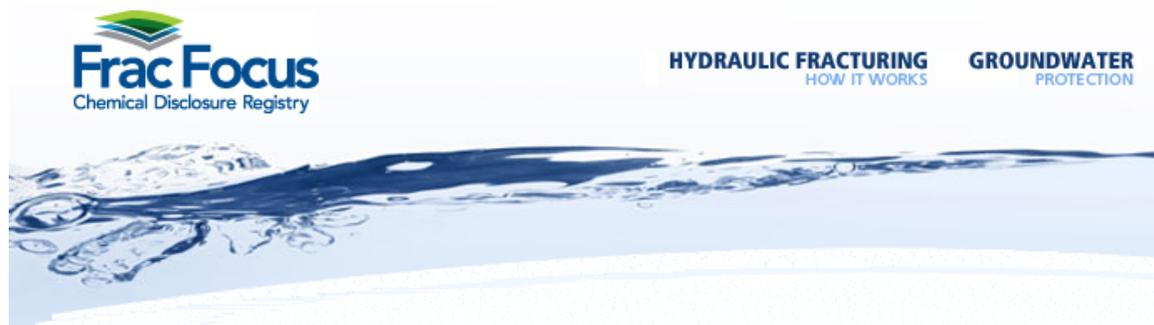
STATUS REPORT

Anthracene		120-12-7
Aromatic oil		
9,10-Anthracenedione, 2-ethyl	2-Ethylanthracene-9,10-dione	84-51-5
Azobenzene		103-33-3
Benz(e)acenaphthylene	Acephenanthrylene	201-06-9
Benzaldehyde, 3-hydroxyl-4-methoxy	3-Hydroxy-4-methoxy-benzaldehyde	621-59-0
Benz(a)anthracene		56-55-3
Benzene		71-43-2
Benzene, 1,3-bis(1-methylethenyl)-	1,3-bis(1-methylethenyl)benzene; 1,3-Diisopropenylbenzene	3748-13-8
Benzene, 1,4-bis(1-methylethenyl)-	1,4-Bis(1-methylethenyl)benzene	1605-18-1
Benzenediamine, N,N'-diphenyl-	N,N'-Diphenyl-p-phenylenediamine	74-31-7

Download as: [TSV](#) [Excel](#) [SDF](#)

ID	Preferred Name	CAS-RN	QC Level	Number of Sources	PubChem Data Source Count
	Azobenzene	103-33-3			
	N,N'-Diphenyl-p-phenylenediamine	74-31-7			
	1,3-Diisopropenylbenzene	3748-13-8			
	Benzene-D6	1076-43-3			
	1,4-Bis(1-methylethenyl)benzene	1605-18-1			
	Benzene	71-43-2			
	2-Ethylanthracene-9,10-dione	84-51-5			
	3-Hydroxy-4-methoxy-benzaldehyde	621-59-0			
	2,6-Anthracenedisulfonic acid, 9,10-dihydro-9,10-dioxo-	84-50-4			
	Acephenanthrylene	201-06-9			

What about these chemicals????

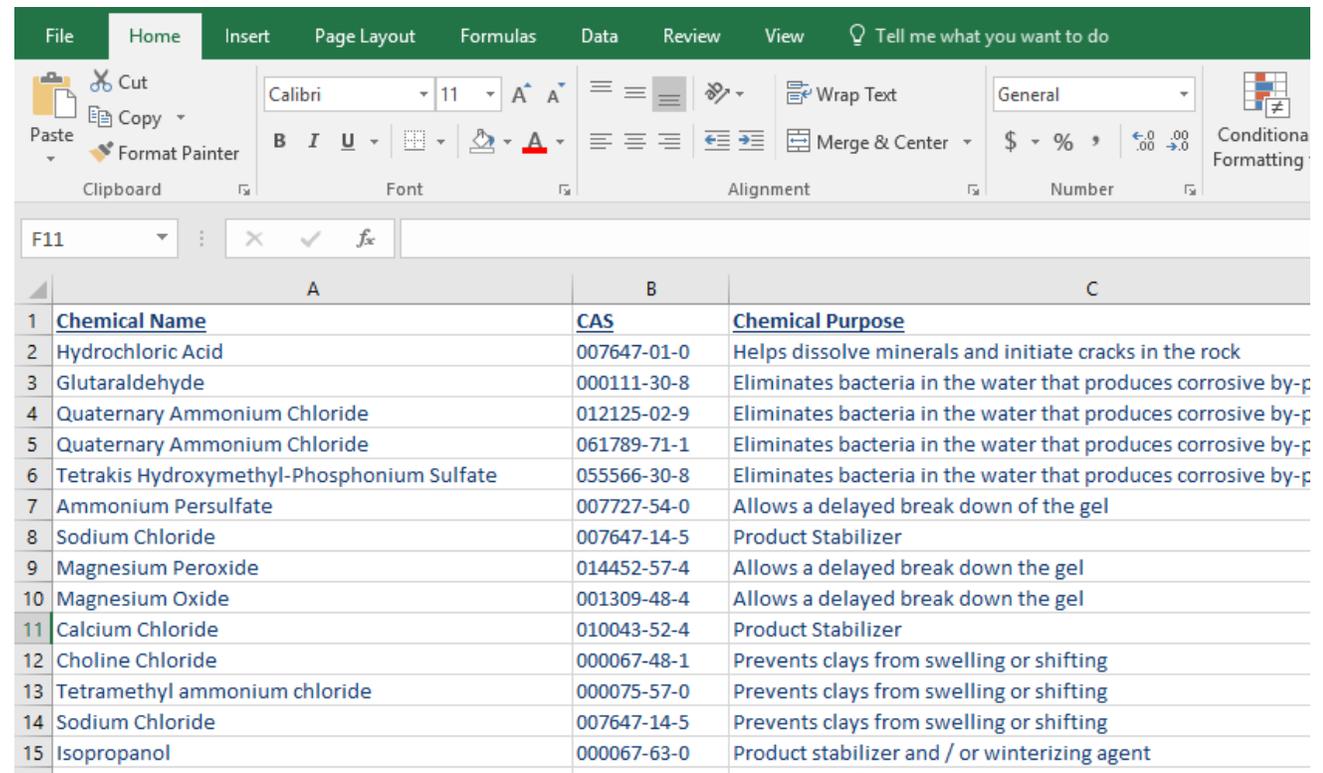


What Chemicals Are Used

As previously noted, chemicals perform many functions in a hydraulic fracturing job. Although there are dozens to hundreds of chemicals which could be used as additives, there are a limited number which are routinely used in hydraulic fracturing.

The following is a list of the chemicals used most often. This chart is sorted alphabetically by the Product Function to make it easier for you to compare to the fracturing records .

<u>Chemical Name</u>	<u>CAS</u>	<u>Chemical Purpose</u>	<u>Product Function</u>
Hydrochloric Acid	007647-01-0	Helps dissolve minerals and initiate cracks in the rock	Acid
Glutaraldehyde	000111-30-8	Eliminates bacteria in the water that produces corrosive by-products	Biocide
Quaternary Ammonium Chloride	012125-02-9	Eliminates bacteria in the water that produces corrosive by-products	Biocide
Quaternary Ammonium Chloride	061789-71-1	Eliminates bacteria in the water that produces corrosive by-products	Biocide



	A	B	C
1	Chemical Name	CAS	Chemical Purpose
2	Hydrochloric Acid	007647-01-0	Helps dissolve minerals and initiate cracks in the rock
3	Glutaraldehyde	000111-30-8	Eliminates bacteria in the water that produces corrosive by-p
4	Quaternary Ammonium Chloride	012125-02-9	Eliminates bacteria in the water that produces corrosive by-p
5	Quaternary Ammonium Chloride	061789-71-1	Eliminates bacteria in the water that produces corrosive by-p
6	Tetrakis Hydroxymethyl-Phosphonium Sulfate	055566-30-8	Eliminates bacteria in the water that produces corrosive by-p
7	Ammonium Persulfate	007727-54-0	Allows a delayed break down of the gel
8	Sodium Chloride	007647-14-5	Product Stabilizer
9	Magnesium Peroxide	014452-57-4	Allows a delayed break down the gel
10	Magnesium Oxide	001309-48-4	Allows a delayed break down the gel
11	Calcium Chloride	010043-52-4	Product Stabilizer
12	Choline Chloride	000067-48-1	Prevents clays from swelling or shifting
13	Tetramethyl ammonium chloride	000075-57-0	Prevents clays from swelling or shifting
14	Sodium Chloride	007647-14-5	Prevents clays from swelling or shifting
15	Isopropanol	000067-63-0	Product stabilizer and / or winterizing agent

What about these chemicals????

Batch Search

Please enter one identifier per line 

Select Input Type(s)

- Chemical Name
- CAS-RN
- InChIKey
- DSSTox Substance ID
- Exact Molecular Formula 

Enter Identifiers to Search

p07647-01-0
000111-30-8
012125-02-9
061789-71-1
055566-30-8
007727-54-0
007647-14-5
014452-57-4
001309-48-4
010043-52-4

Display All Chemicals

Download Chemical Data

What about these chemicals????

Select Output Format

Customize Results

Select All

Chemical Identifiers	Structures	Intrinsic And Predicted Properties
<input checked="" type="checkbox"/> Chemical Name	<input type="checkbox"/> Mol File	<input type="checkbox"/> Molecular Formula
<input checked="" type="checkbox"/> DTXSID	<input type="checkbox"/> SMILES	<input type="checkbox"/> Average Mass
<input checked="" type="checkbox"/> CAS-RN	<input type="checkbox"/> InChI String	<input type="checkbox"/> Monoisotopic Mass
<input type="checkbox"/> InChIKey		<input checked="" type="checkbox"/> OPERA Model Predictions
<input type="checkbox"/> IUPAC Name		<input type="checkbox"/> TEST Model Predictions

Metadata	Presence In Lists
<input type="checkbox"/> Curation Level Details	<input type="checkbox"/> Algal Toxins
<input type="checkbox"/> Data Sources	<input type="checkbox"/> ATSDR Toxic Substances Portal Chemical List
<input checked="" type="checkbox"/> Assay Hit Count	<input type="checkbox"/> Bisphenol Compounds
<input type="checkbox"/> Include links to ACToR reports - SLOW! (BETA)	<input type="checkbox"/>
<input checked="" type="checkbox"/> NHANES/Predicted Exposure	California Office of Environmental Health Hazard Assessment
<input checked="" type="checkbox"/> Include ToxVal Data Availability	<input type="checkbox"/> DNT Screening Library
	<input type="checkbox"/> Drinking Water Suspects, KWR Water, Netherlands

What about these chemicals????

A	B	C	D	E	F	G	H	I	J
INPUT	DTXSID	PREFERRED NAME	CASRN	TOXCAST	TOXCAST	EXPOCAST	EXPOCAST	NHANES	TOXVAL DATA
007647-01-0	DTXSID2020711	Hydrochloric acid	7647-01-0	-	-	-	-	-	Y
000111-30-8	DTXSID6025355	Glutaraldehyde	111-30-8	12.86	71/552	Y	2.03e-05	-	Y
012125-02-9	DTXSID0020078	Ammonium chloride	12125-02-9	-	-	-	-	-	Y
061789-71-1	Checksum Failed	-							
055566-30-8	DTXSID0021331	Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	4.71	13/276	Y	3.47e-08	-	Y
007727-54-0	DTXSID9029691	Diammonium peroxydisulfate	7727-54-0	0.88	1/113	-	-	-	Y
007647-14-5	DTXSID3021271	Sodium chloride	7647-14-5	-	-	-	-	-	Y
014452-57-4	DTXSID9049667	Magnesium peroxide	14452-57-4	-	-	-	-	-	Y
001309-48-4	DTXSID9049665	Magnesium oxide	1309-48-4	-	-	-	-	-	Y
010043-52-4	DTXSID5020235	Calcium chloride	10043-52-4	0.88	1/113	Y	9.45e-05	-	Y
000067-48-1	DTXSID4020325	Choline chloride	67-48-1	0.0	0/113	Y	4.94e-07	-	Y
000075-57-0	DTXSID6021749	Tetramethylammonium chloride	75-57-0	0.0	0/113	Y	5.33e-08	-	Y
007647-14-5	DTXSID3021271	Sodium chloride	7647-14-5	-	-	-	-	-	Y
000067-63-0	DTXSID7020762	Isopropanol	67-63-0	9.73	11/113	Y	4.8e-05	-	Y
000067-56-1	DTXSID2021731	Methanol	67-56-1	0.0	0/113	Y	3.01e-05	-	Y
000064-18-6	DTXSID2024115	Formic acid	64-18-6	-	-	-	-	-	Y
000075-07-0	DTXSID5039224	Acetaldehyde	75-07-0	22.1	61/276	Y	2.57e-06	-	Y
064741-85-1	DTXSID0028169	Raffinates, petroleum, sorption process	64741-85-1	-	-	-	-	-	-
064742-47-8	DTXSID8028212	Distillates, petroleum, hydrotreated light	64742-47-8	-	-	-	-	-	Y

Quaternary ammonium compounds, benzylcoco alkyldimethyl, chlorides
61789-71-7 | DTXSID6029381

Curating Chemistry Data is painful

A	B	C
INPUT	DTXSID	PREFERRED NAME
007647-01-0	DTXSID2020711	Hydrochloric acid
000111-30-8	DTXSID6025355	Glutaraldehyde
012125-02-9	DTXSID0020078	Ammonium chloride
061789-71-1	Checksum Failed	-
055566-30-8	DTXSID0021331	Tetrakis(hydroxymethyl)ph
007727-54-0	DTXSID9029691	Diammonium peroxydisulf
007647-14-5	DTXSID3021271	Sodium chloride
014452-57-4	DTXSID9049667	Magnesium peroxide

<u>Chemical Name</u>	<u>CAS</u>	<u>Chemical Purpose</u>	<u>Product Fur</u>
Hydrochloric Acid	007647-01-0	Helps dissolve minerals and initiate cracks in the rock	Acid
Glutaraldehyde	000111-30-8	Eliminates bacteria in the water that produces corrosive by-products	Biocide
Quaternary Ammonium Chloride	012125-02-9	Eliminates bacteria in the water that produces corrosive by-products	Biocide
Quaternary Ammonium Chloride	061789-71-1	Eliminates bacteria in the water that produces corrosive by-products	Biocide
Tetrakis Hydroxymethyl	055566-30-8	Eliminates bacteria in the water that produces	Biocide

Quaternary ammonium compounds, benzylcoco alkyldimethyl, chlorides
61789-71-7 | DTXSID6029381

Compare CAS Numbers:
61789-71-1 (**FAIL**) versus 61789-71-7 (**OCR failure?**)

What about these chemicals????

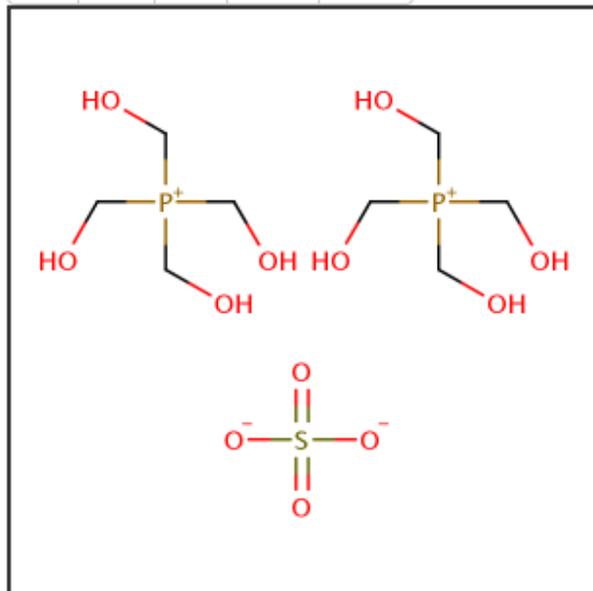
A	B	C	D	E	F	G	H	I	J
INPUT	DTXSID	PREFERRED NAME	CASRN	TOXCAST	TOXCAST	EXPOCAST	EXPOCAST	NHANES	TOXVAL DATA
007647-01-0	DTXSID2020711	Hydrochloric acid	7647-01-0	-	-	-	-	-	Y
000111-30-8	DTXSID6025355	Glutaraldehyde	111-30-8	12.86	71/552	Y	2.03e-05	-	Y
012125-02-9	DTXSID0020078	Ammonium chloride	12125-02-9	-	-	-	-	-	Y
061789-71-1	Checksum Failed								
055566-30-8	DTXSID0021331	Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	4.71	13/276	Y	3.47e-08	-	Y
007727-54-0	DTXSID9029691	Diammonium peroxydisulfate	7727-54-0	0.88	1/113	-	-	-	Y
007647-14-5	DTXSID3021271	Sodium chloride	7647-14-5	-	-	-	-	-	Y
014452-57-4	DTXSID9049667	Magnesium peroxide	14452-57-4	-	-	-	-	-	Y
001309-48-4	DTXSID9049665	Magnesium oxide	1309-48-4	-	-	-	-	-	Y
010043-52-4	DTXSID5020235	Calcium chloride	10043-52-4	0.88	1/113	Y	9.45e-05	-	Y
000067-48-1	DTXSID4020325	Choline chloride	67-48-1	0.0	0/113	Y	4.94e-07	-	Y
000075-57-0	DTXSID6021749	Tetramethylammonium chloride	75-57-0	0.0	0/113	Y	5.33e-08	-	Y
007647-14-5	DTXSID3021271	Sodium chloride	7647-14-5	-	-	-	-	-	Y
000067-63-0	DTXSID7020762	Isopropanol	67-63-0	9.73	11/113	Y	4.8e-05	-	Y
000067-56-1	DTXSID2021731	Methanol	67-56-1	0.0	0/113	Y	3.01e-05	-	Y
000064-18-6	DTXSID2024115	Formic acid	64-18-6	-	-	-	-	-	Y
000075-07-0	DTXSID5039224	Acetaldehyde	75-07-0	22.1	61/276	Y	2.57e-06	-	Y
064741-85-1	DTXSID0028169	Raffinates, petroleum, sorption process	64741-85-1	-	-	-	-	-	-
064742-47-8	DTXSID8028212	Distillates, petroleum, hydrotreated light	64742-47-8	-	-	-	-	-	Y

Single Click Navigation into the Chemical

Tetrakis(hydroxymethyl)phosphonium sulfate

55566-30-8 | DTXSID0021331

© Searched by CAS-RN: Found 1 result for '55566-30-8'.



Intrinsic Properties

Structural Identifiers

Related Compounds

Presence in Lists

Record Information

Citation

U.S. Environmental Protection Agency. Chemistry Dashboard. <https://comptox.epa.gov/dashboard/DTXSID0021331> (accessed October 16, 2017), Tetrakis(hydroxymethyl)phosphonium sulfate



Data Quality

Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers

Data for Download

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

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	DTXS ID
316388891	20404	DTXS ID30873143
316388890	10142816	DTXS ID70873142
316388889	50742127	DTXS ID40873139
316388888	19073841	DTXS ID20873137
316388887	11505215	DTXS ID00873135
316388886	25021861	DTXS ID80873133
316388885	2784427	DTXS ID60873131
316388884	6731	DTXS ID00873130

[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.

	A	B	
1	casrn	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



Future Work

- Continue expansion and curation of data and types.
- Provide “**programmatic access**” to all data – connect to other Agency resources and allow other scientists to integrate their scientific applications.
- Continue to assemble and enhance chemical lists and data for specific projects. Make available to Agency researchers and for public use.
- Make new modules public – “Generalized Read Across”, “EcoTox data”



Conclusion

- Chemistry Dashboard for ~760,000 chemicals and associated data
 - Search for single chemical or batch-based searching
 - A focus on data curation and quality
- An **Integration Hub** – *in vitro* HTS, *in vivo* hazard toxicity, experimental and predicted physchem and fate and transport data
 - Transparency in predictions and access to Open Data
- Data downloads allows for reuse in other systems and integration of resources to support research



Acknowledgments

- The collective work of many
 - Chris Grulke
 - Andrew McEachran
 - Nancy Baker
 - Kathie Dionisio
 - Katharine Phillips
 - Kristin Isaacs
 - Jon Sobus
 - John Wambaugh
 - Richard Judson
 - Ann Richard
- Many colleagues across the agency

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