

The EPA CompTox Chemistry Dashboard and Underpinning Software Architecture – a platform for data integration for environmental chemistry data

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*August 2017
ACS Fall Meeting, Washington, DC*

PRIMARY GOALS

- Deliver a web-based application serving up the chemistry related data used by our team
- Provide public access to the results of over a decade of curation work reviewing environmental chemistry data
- Provide access to the results of our QSAR modeling work
- 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 cheminformatics architecture to serve as a high quality chemical foundation for all NCCT tools and data

The CompTox Chemistry Dashboard: An Overview

- **A publicly accessible website** delivering access:
 - ~760,000 chemicals and related property data
 - Links to other agency websites and public data resources
 - “Literature” searches for chemicals using public resources
 - Integration to “biological assay data” for 1000s of chemicals
 - Information regarding consumer products containing chemicals
 - “Batch searching” for thousands of chemicals
- Day-to-day curation efforts for data quality

Our Chemistry Content



Mutation Research/Fundamental and
Molecular Mechanisms of Mutagenesis

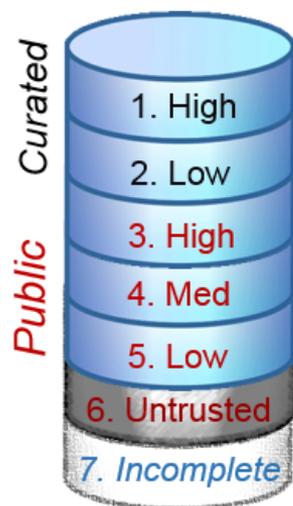
Volume 499, Issue 1, 29 January 2002, Pages 27-52



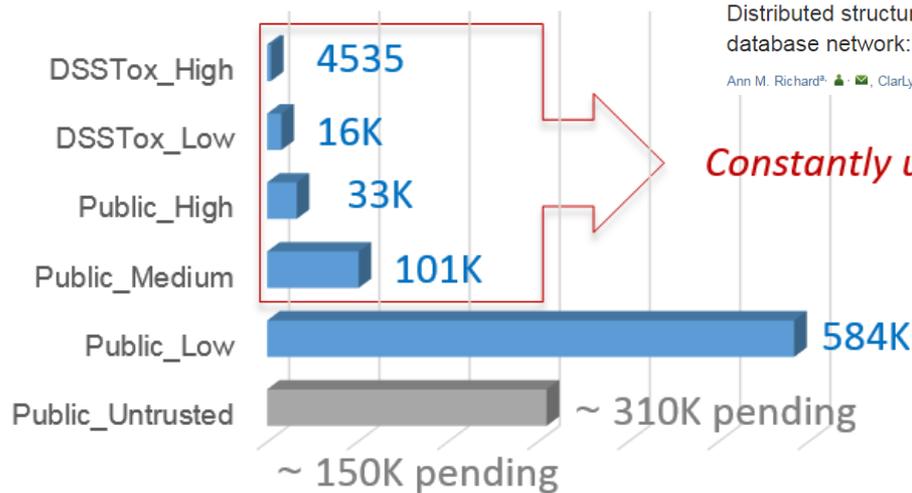
Mutation Research Frontiers

Distributed structure-searchable toxicity (DSSTox) public
database network: a proposal

Ann M. Richard^a,  , ClarLynda R. Williams^{a, b}



QC Level Totals

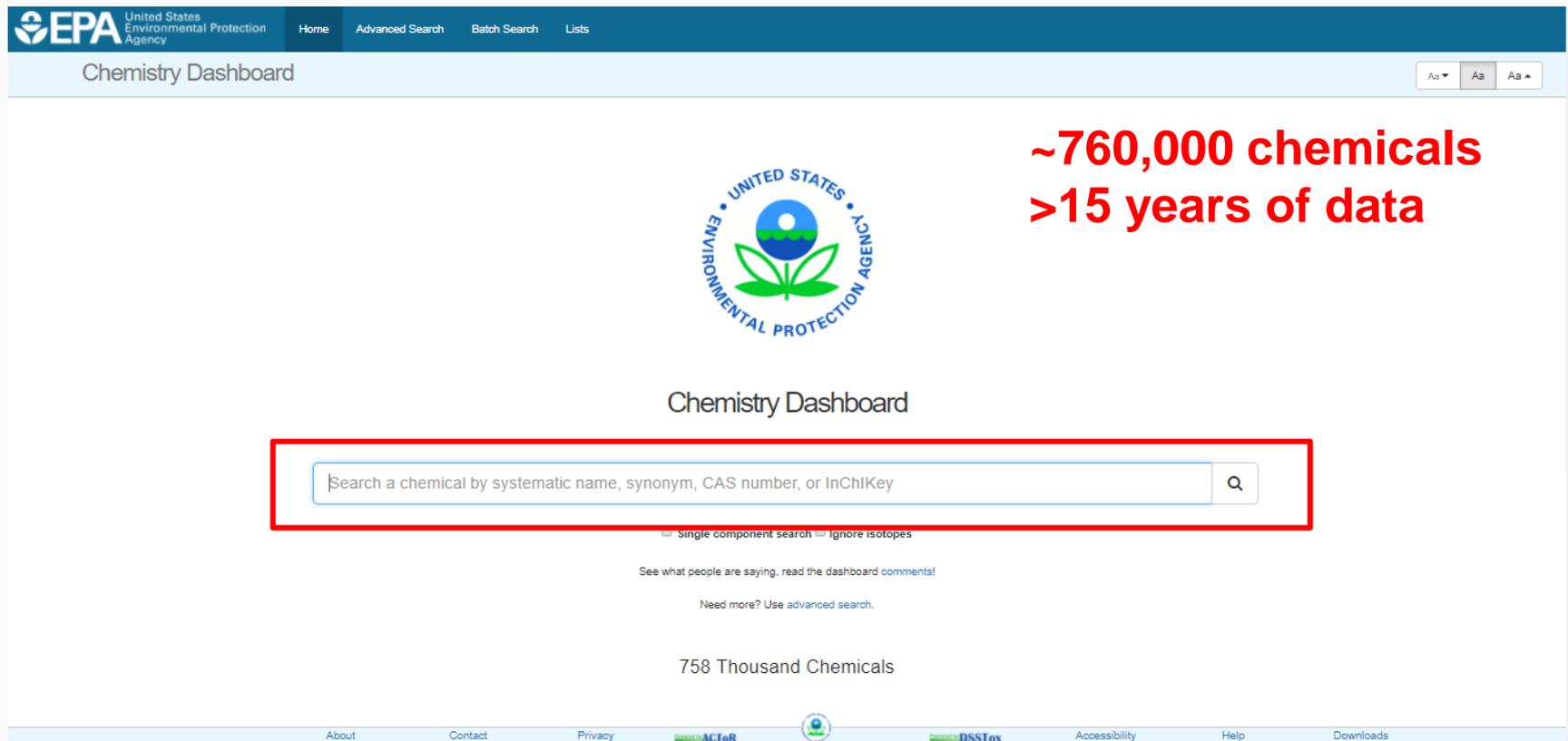


QC Levels

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>



United States Environmental Protection Agency

Home Advanced Search Batch Search Lists

Chemistry Dashboard

~760,000 chemicals
>15 years of data

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

Chemistry Dashboard

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!

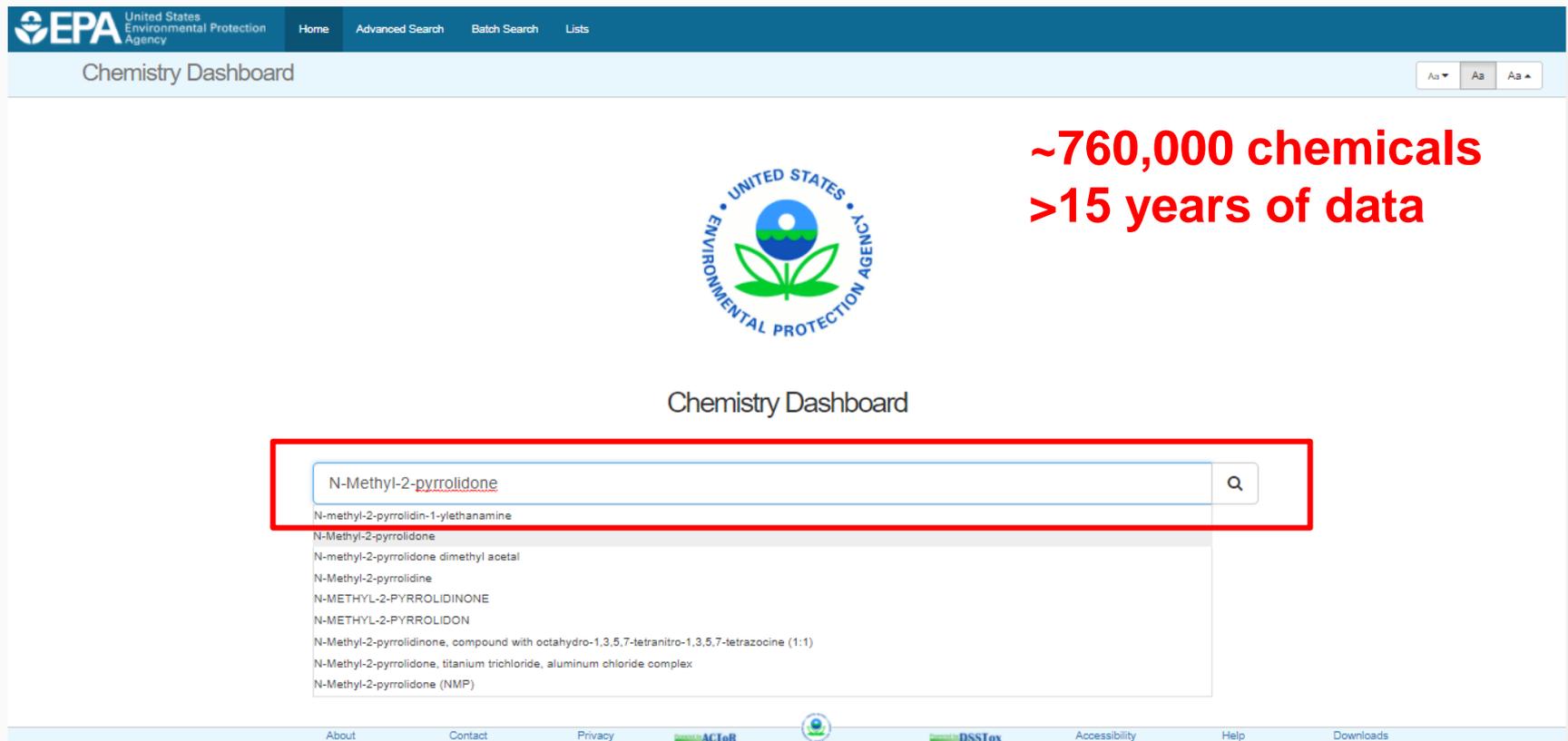
Need more? Use advanced search.

758 Thousand Chemicals

About Contact Privacy ACToR DSSTox Accessibility Help Downloads

Comptox Chemistry Dashboard

<https://comptox.epa.gov>



Chemistry Dashboard

~760,000 chemicals
>15 years of data

Chemistry Dashboard

N-Methyl-2-pyrrolidone

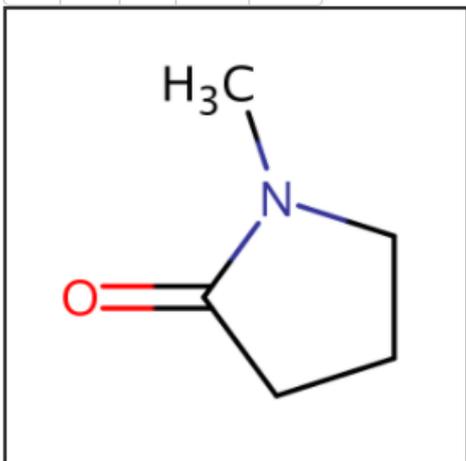
- N-methyl-2-pyrrolidin-1-ylethanamine
- N-Methyl-2-pyrrolidone
- N-methyl-2-pyrrolidone dimethyl acetal
- N-Methyl-2-pyrrolidine
- N-METHYL-2-PYRROLIDINONE
- N-METHYL-2-PYRROLIDON
- N-Methyl-2-pyrrolidinone, compound with octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (1:1)
- N-Methyl-2-pyrrolidone,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

About Contact Privacy ACToR DSSTox Accessibility Help Downloads

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

Find All Chemicals 



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:

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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	-	-	-
Molar Weight	-	62.0 (1)	-	62.0	-	-	g/mol

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

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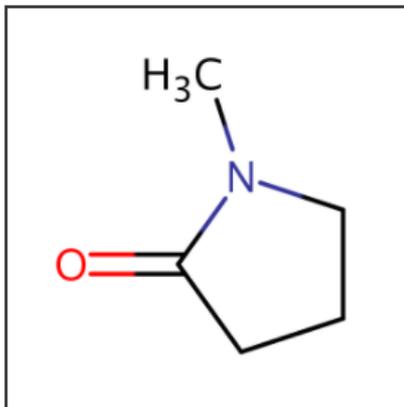
External Links

- Solubility
- Melting Point
- Boiling Point
- LogP (Octanol-water partition coefficient)
- Atmospheric Hydroxylation Rate
- LogBCF (Bioconcentration Factor)
- Biodegradation Half-life
- Henry's Law Constant
- Fish Biotransformation Half-life
- LogKOA (Octanol/Air Partition Coefficient)
- LogKOC (Soil Adsorption Coefficient)
- Vapor Pressure

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

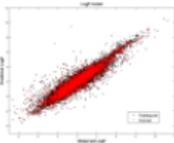
Predicted value: -0.300

Global applicability domain: inside ⓘ

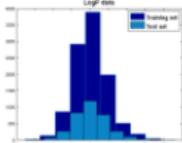
Local applicability domain index: 0.88 ⓘ

Confidence level: 0.81 ⓘ

Model Performance



Q2



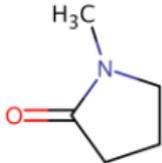
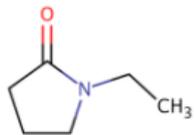
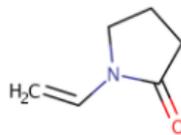
Q2

Weighted KNN model

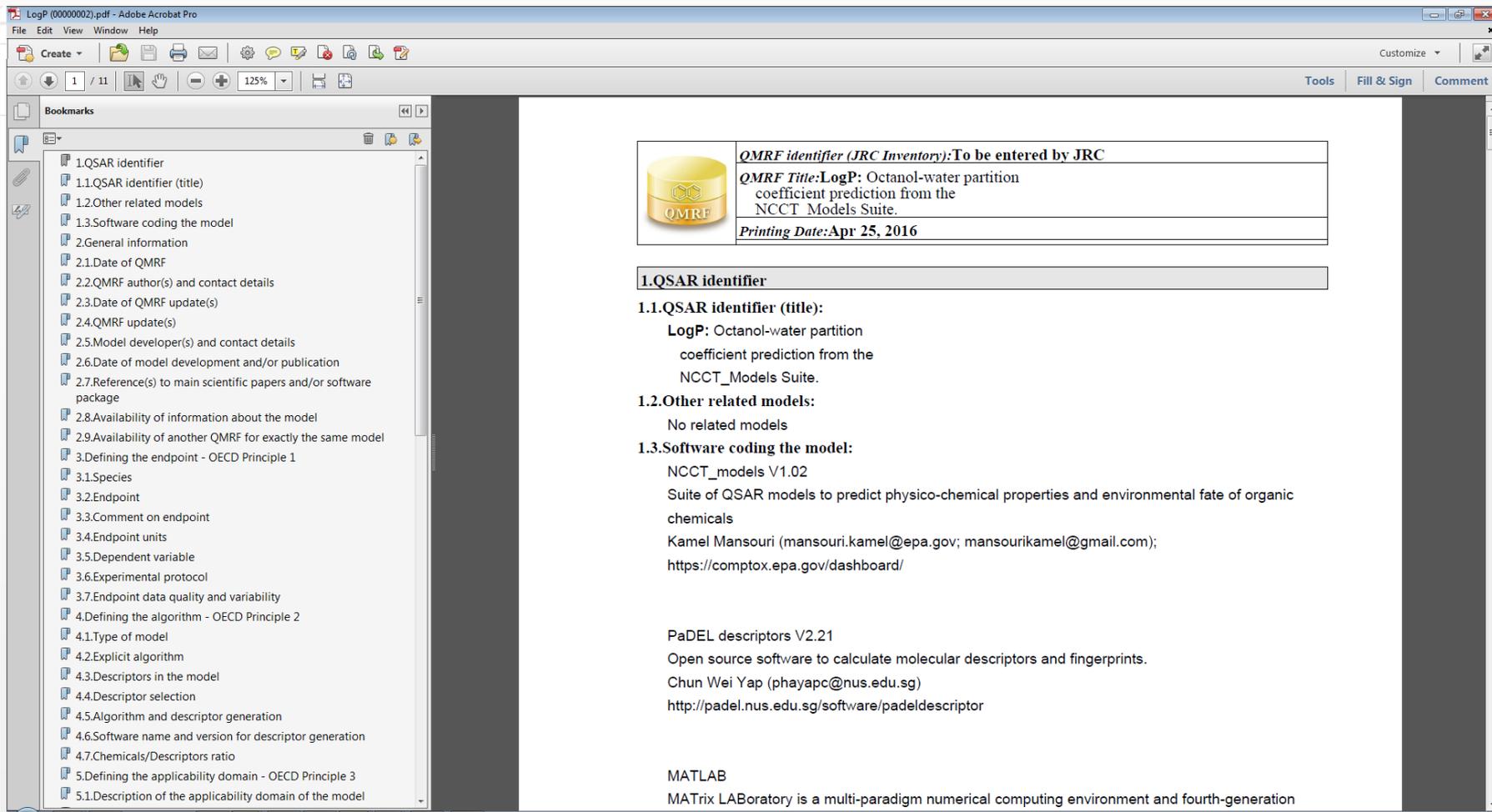
QMRf

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

 <p>N-Methyl-2-pyrrolidone Measured: -0.380 Predicted: -0.300</p>	 <p>Prolinal Measured: -0.320 Predicted: -0.226</p>	 <p>1-Ethyl-2-pyrrolidinone Measured: -0.0400 Predicted: -0.211</p>	 <p>N-Vinyl-2-pyrrolidone Measured: 0.37 Predicted: 2.65e-01</p>
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QSAR Modeling Reporting Format



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 QMRP
 - 2.2. QMRP author(s) and contact details
 - 2.3. Date of QMRP update(s)
 - 2.4. QMRP 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 QMRP 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

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

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

Toxicity Values

Bioavailability Metric

Exposure Limit

Point Of Departure

Regulatory Toxicity Value

Effect Level

Misc Hazard Information

Screening Level

Uncertainty Factor

Download as:

TSV

Excel

Type	Subtype	Value	Units	Study Type	Exposure Route	Study Duration	Species	Media	Details	Source
TD50	-	20.7	mM/kg-day	-	-	-	-	-	DSSTox C...	ACToR
TD50	-	2050	mg/kg-day	-	-	-	-	-	DSSTox C...	ACToR
LEL	systemic	619	mg/kg-day	subchronic	oral	subchronic	mouse	-	Study ID: ...	ToxRefDB
NEL	systemic	277	mg/kg-day	subchronic	oral	subchronic	mouse	-	Study ID: ...	ToxRefDB
LEL	systemic	25.0	mg/kg-day	subchronic	oral	subchronic	dog	-	Study ID: ...	ToxRefDB
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:

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
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/...

[Chemical Properties](#)

[Env. Fate/Transport](#)

[Toxicity Values \(Beta\)](#)

[ADME \(Beta\)](#)

[Exposure](#)

[Bioassays](#)

[Similar Molecules \(Beta\)](#)

[Synonyms](#)

[Literature](#)

[External Links](#)

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

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

External Links

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](#)

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[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 ...

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

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[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

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

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Synonyms

Literature

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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

ng Articles

rrolidone" OR "N-methylpyrrolidone"

Search and Count

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

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Similar Molecules (Beta)

Synonyms

Literature

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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	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	23337464	2013	Biomonitoring of exposure to N-methyl-2-pyrrolidone in workers of the automobile industry.
0	0	0	0	19875680	2009	Quantitative risk analysis for N-methyl pyrrolidone using physiologically based pharmacokinetic and benchmark dos...
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)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

External Links

Select Term:

Exposure ▼

Retrieve Articles

0 Articles

Add additional query terms to filter abstracts:

developmental

reproductive

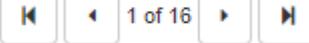
occupational

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.

Links to Other Resources

General

-  EPA Substance Re...
-  NIST Chemistry W...
-  Household Product...
-  PubChem
-  Chempider
-  CPCat
-  DrugBank
-  HMDB
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  Chemical Vendors
-  Consumer Product...

Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  EPA
-  GHS
-  HSDB
-  ToxCast Dashboar...
-  LactMed
-  ACToR PDF Report
-  International Toxicit...

Publications

-  Toxline
-  Environmental Heal...
-  NIEHS
-  National Toxicology...
-  Google Books
-  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 

Quick Search

Product, Manufacturer etc...

Advanced Search ▶

Browse by Category

- Inside the Home
- Home Maintenance
- Personal Care
- Landscape/Yard
- Arts & Crafts
- Pet Care
- Pesticides
- Auto Products
- Home Office
- Commercial / Institutional

Browse A-Z

- Products Names
- Types of Products
- Manufacturers
- Ingredients

Support

- About the Database
- FAQ
- Product Recalls
- Help

 **ChemHAT.org**
Chemical Hazard and Alternatives Toolbox

English | Español

ECHA
EUROPEAN CHEMICALS AGENCY

Search the ECHA Website

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[About Us](#) [Regulations](#) [Addressing Chemicals of Concern](#) [Information on Chemicals](#) [Chemicals in our Life](#) [Support](#)

N-methylpyrrolidone

CAS: 872-50-4

How can this ch

- Acute (Short Term)**
 -  **Irritates the Eyes** - Can irritate or serious damage to the eye.
- Chronic (Long Term)**
 -  **Birth Defects** - Can cause developing child including defects, low birth weight, biological or behavioral abnormalities appear as the child grows.
 -  **Other Health Effects** - (Serious damage on contact with skin or ingestion).

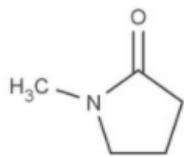
ECHA > Substance Information > 1-methyl-2-pyrrolidone 

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]  

<p>Substance identity ⓘ</p> <p>EC / List no.: 212-828-1</p> <p>CAS no.: 872-50-4</p> <p>Mol. formula: C5H9NO</p> <div style="text-align: center;">  </div>	<p>Hazard classification & labelling ⓘ</p> <div style="text-align: center;">  </div> <p><i>Danger!</i> 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>Properties of concern ⓘ</p> <div style="text-align: center;">  </div> <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.

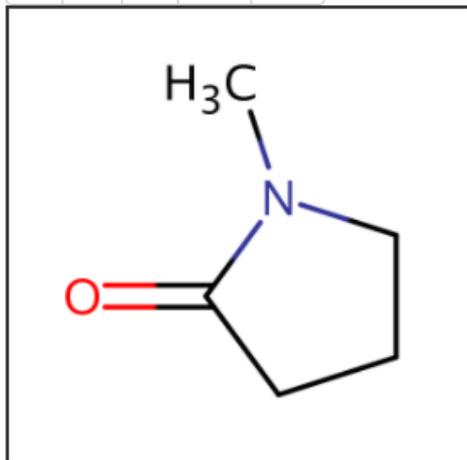
This substance is used by consumers, by professional workers (widespread uses), in formulation or re-

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

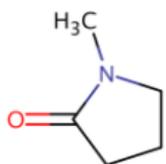
Hide Multicomponent Chemicals



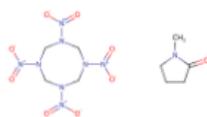
Aa ▼

Aa

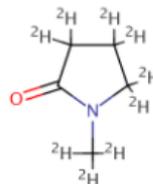
Aa ▲



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



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



1-(²H³)Met...
185964-60-7

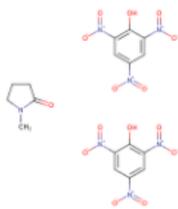


HCl

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



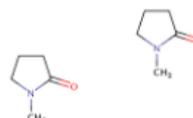
Sulfuric acid--1-methylpyrrolidin-2-on...
80997-96-2



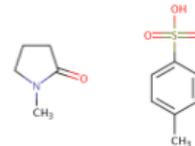
1-Methylpyrrolidin-2-one--2,4,6-trinitro...
61727-04-6



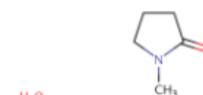
Nitric acid--1-methylpyrrolidin-2-one (...
918666-25-8



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



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



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



Not just structures – “UVCBs”

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

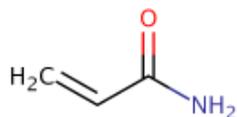
U.S. Environmental Protection Agency. Chemistry Dashboard. <https://comptox.epa.gov/dashboard/DTXSID1049722> (accessed February 12, 2017), Poly (acrylamide-co-acrylic acid), partial sodium salt

Data Quality **80%**

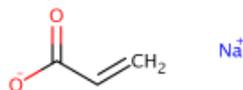
Manually curated and no conflicts in multiple public sources

Related Chemicals

Found 2 chemicals



Acrylamide
79-06-1



2-Propenoic acid, sodium salt
7446-81-3

- 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

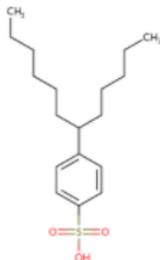
i Searched by Synonym: Found 1 result for
'Linear alkylbenzene sulfonate'.

Presence in Lists

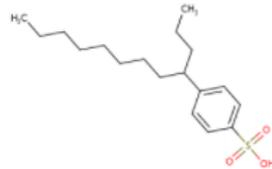
Surfactant List Screened in Swiss Wastewater (2014)

Surfactant List Screened in Swiss Wastewater (2014)

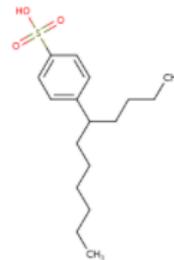
EAWAGSURF is a list of surfactants screened in Swiss wastewater effluents as part of a 2014 study. Structures/mixtures are being progressively curated and linked (Schymanski/Williams). Further details in Schymanski et al 2014, DOI: 10.1021/es4044374



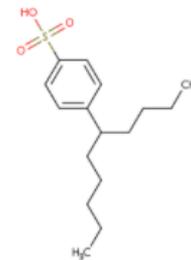
4-(Dodecan-6-yl)benzene-1-sulfon...
23003-92-1



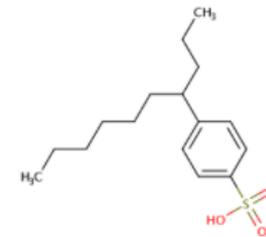
4-(dodecan-4-yl)benzene-1-sulfoni...
NOCAS_862870



C11-LAS
NOCAS_881097



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



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

Batch Searching for Data for Thousands of Chemicals

- What are these chemicals?

**Chemicals Used in the Hydraulic Fracturing Process in Pennsylvania
Prepared by the Department of Environmental Protection
Bureau of Oil and Gas Management**

Updated June 10, 2010

Chemical	Product Name
2,2-Dibromo-3-Nitrilopropionamide	Bio Clear 1000/Bio Clear 2000/ Bio-Clear 200/BioRid20L/ EC6116A
2-methyl-4-isothiazolin-3-one	X-Cide 207
5-chloro-2-methyl-4-isothiazolin-3-one	X-Cide 207
Acetic Acid	Fe-1A Acidizing Composition/ Packer Inhibitor
Acetic Anhydride	Fe-1A Acidizing Composition
Acetylene	GT&S Inc./ Airco
Alcohol Ethoxylated	C12-16 NE-200
Alkyl benzene sulfonic acid	Tetrolite AW0007/ FR-46
Ammonia (aqueous)	FAW-5
Ammonium Bifluoride	ABF 37%
Ammonium Persulfate	AP Break
Ammonium Bisulfite	Techni-Hib 604/ Fe OXCLEAR/ Packer Inhibitor
Ammonium chloride	Salt Inhibitor
Ammonium Salt (alkylpolyether	

Batch Searching for Data for Thousands of Chemicals

Select Input Type(s)

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

Enter Identifiers to Search

Sodium L-glutamate
4-Hydroxy-3-nitrophenylarsonic acid
4-Nitro-1,2-phenylenediamine
Methoxypromazine
1-Phenyl-3-methyl-5-pyrazolone
1-Phenyl-2-thiourea
Phenylbutazone
1,4-Benzenediamine
Prednisolone
Probenecid

Display All Chemicals Download Chemical Data

Select Output Format

Excel ▼

Customize Results

- Select All

Chemical Identifiers	Structures	Intrinsic 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 type="checkbox"/> CAS-RN	<input type="checkbox"/> InChI String	<input type="checkbox"/> Monoisotopic Mass
<input type="checkbox"/> InChIKey		<input type="checkbox"/> OPERA and TEST Model Predictions
<input type="checkbox"/> IUPAC Name		

Access to associated data for review, modeling & download

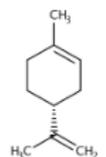
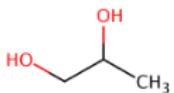
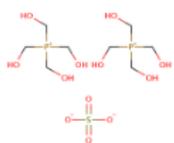
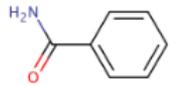
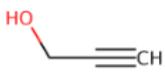
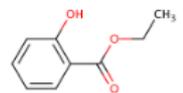
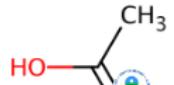
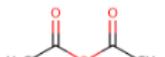
 United States Environmental Protection Agency

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Chemistry Dashboard

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 <p>D-Limonene 5989-27-5</p>	$K^+ Cl^-$ <p>Potassium chloride 7447-40-7</p>	 <p>1,2-Propylene glycol 57-55-6</p>	$Na^+ O^- C(=O)OH$ <p>Sodium bicarbonate 144-55-8</p>	 <p>Tetrakis(hydroxymethyl)phospho... 55566-30-8</p>	
 <p>Benzamide 55-21-0</p>	H_3C-OH <p>Methanol 67-56-1</p>	 <p>1-Butanol 71-36-3</p>	 <p>Propargyl alcohol 107-19-7</p>	 <p>Ethyl salicylate 118-61-6</p>	
 <p>About</p>	 <p>Contact</p>	 <p>Privacy</p>	 <p>ACToR</p>	 <p>DSSTox</p>	
			Accessibility	Help	Downloads

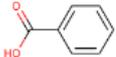
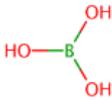
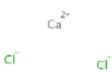
Access to associated data for review, modeling & download

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Chemistry Dashboard

Searched by List: Found 64 results.

Download as:

ID ↑↓	Structure	Preferred Name ↑↓	CAS-RN ↑↓	QC Level ↑↓	CPCat C..	Number...	PubChe...	Monoisotopic M...	
DTXSID0020078 <small>cf</small>		Ammonium chloride	12125-02-9	DSSTox High	561	28	82	53.003227	<input type="checkbox"/>
DTXSID6020143 ToxCast™		Benzoic acid	65-85-0	DSSTox High	87	70	441	122.036779	<input type="checkbox"/>
DTXSID1020194 ToxCast™		Boric acid	10043-35-3	DSSTox High	792	51	142	62.017524	<input type="checkbox"/>
DTXSID5020235 ToxCast™		Calcium chloride	10043-52-4	DSSTox High	294	33	81	109.900296	<input type="checkbox"/>

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- From chemical names to chemical data



EPA
United States Environmental Protection Agency

ATSDR
Agency for Toxic Substances and Hazardous Waste Investigation

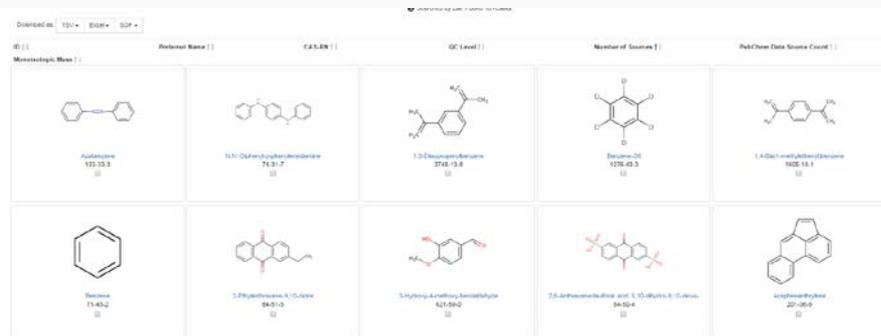
NIOSH
National Institute for Occupational Safety and Health

CDC
Centers for Disease Control and Prevention

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

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-hydroxy-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
1,4-Benzenediamine, N,N'-diphenyl-	N,N'-Diphenyl-p-phenylenediamine	74-31-7



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Microscopic View

Reference Name	CASRN	QC Level	Number of Sources	PubChem Data Source Count
Azobenzene	103-33-3	II	12	12
1,3-Diphenylisobenzofuran	74-31-7	II	12	12
1,3-Dioxane	3748-13-8	II	12	12
Stilbene	103-40-3	II	12	12
1,4-Diisopropenylbenzene	1605-18-1	II	12	12
Benzene	71-43-2	II	12	12
1,3-Phenylenediamine	94-30-4	II	12	12
3-Hydroxy-4-methoxybenzaldehyde	621-59-0	II	12	12
2,6-Dibromonitrobenzene and 1,3,5-Trinitro-2,4-Dichlorobenzene	94-30-4	II	12	12
Anthracene	120-12-7	II	12	12

Confidential Business Information under TSCA

Federal Register Notice on Substantiating TSCA CBI claims

On January 19, 2017, EPA announced an interpretation of TSCA section 14 relating to substantiating CBI claims. [Learn More](#)

1 2

CBI is broadly defined as proprietary information, considered confidential to the submitter, the release of which would cause substantial business injury to the owner.

- The dashboard code and data will be deployed in the Office of Pollution Prevention and Toxics (OPPT) supporting CBI data
 - Integrate OPPT CBI data in the database
 - Isolate all internet-based modules for the CBI environment – no external links, no literature searching, no PubChem data etc.
 - Rebuild OPERA models using CBI data (if the models improve can we release without training data?)

JOURNAL OF

CHEMICAL INFORMATION
AND MODELING

Article

pubs.acs.org/jcim

Developing Collaborative QSAR Models Without Sharing Structures

Peter Gedeck,^{*,†} Suzanne Skolnik,[‡] and Stephane Rodde[¶]

[†]Peter Gedeck LLC, 2309 Grove Avenue, Falls Church, Virginia 22046, United States

[‡]Novartis Institute for Biomedical Research, 250 Massachusetts Avenue, Cambridge, Massachusetts 02139, United States

[¶]Novartis Institute for Biomedical Research, Postfach, CH-4002 Basel, Switzerland

SOFTWARE | OPEN ACCESS

eTOXlab, an open source modeling framework for implementing predictive models in production environments

[Pau Carrió](#), [Oriol López](#), [Ferran Sanz](#) and [Manuel Pastor](#) ✉

Journal of Cheminformatics 2015 7:8 | <https://doi.org/10.1186/s13321-015-0058-6> | © Carrió et al.; licensee Springer. 2015

Received: 13 September 2014 | Accepted: 24 February 2015 | Published: 11 March 2015

- Continue expansion and curation of data and types
- Provide “**programmatic access**” to all data – web services and application programming interface
- Continue to assemble and enhance chemical lists and data for specific projects
- Make new modules public – “Generalized Read Across”, “EcoTox data”

- The CompTox Chemistry Dashboard provides access to data for ~760,000 chemicals
- An **Integration Hub** to data – toxicity, environmental, property, bioassay, and expanding
- Data downloads allows for reuse in other systems and integration of resources to support research

Acknowledgments



Antony Williams

US EPA Office of Research and Development

National Center for Computational Toxicology (NCCT)

Williams.Antony@epa.gov

ORCID: <https://orcid.org/0000-0002-2668-4821>