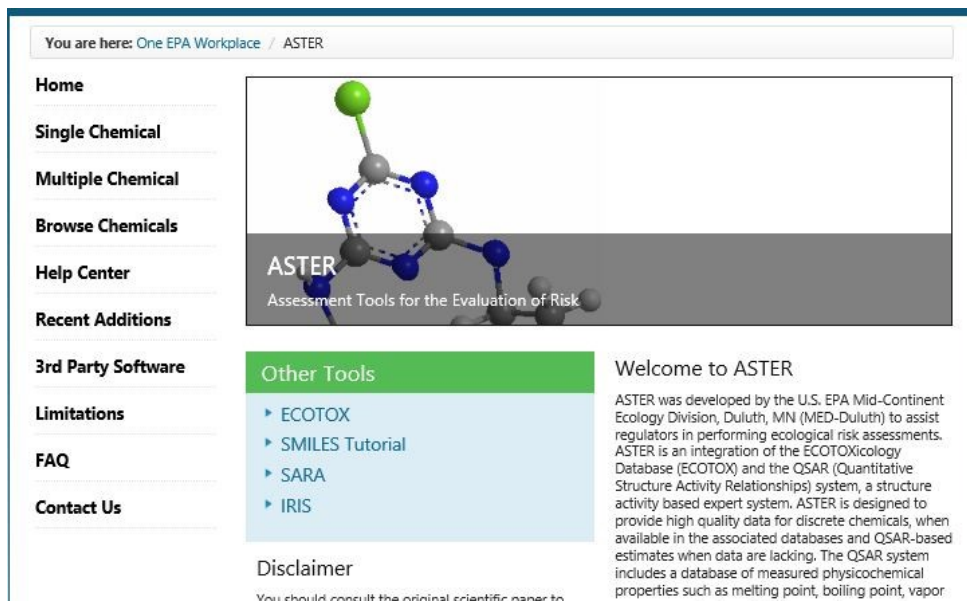


**OVERVIEW:** ASTER (ASsessment Tools for the Evaluation of Risk) was developed at the U.S. EPA Office of Research and Development's Duluth Division (MN), with funding from the U.S. EPA Office of Solid Waste and Emergency Response, and ORD's National Center for Computational Toxicology. The objective was development of an intranet application which could assist EPA in hazard ranking, and for the development of comprehensive risk assessments. ASTER is designed to provide high quality data for discrete chemicals, when available in the associated databases (i.e., ECOTOX Knowledgebase and EcoChem), and QSAR-based estimates when data are lacking. ASTER contains data for 65,659 chemicals with 41,843

structures and ECOTOX data for 12,155 chemicals. Users can search by Chemical Abstract Services (CAS) Registry number, chemical name, or the chemical's structure as represented by a SMILES string. The software allows users to see details on how parameters were calculated or change critical information such as physical/chemical property data or the acute mode of toxic action. Reports are available in either an HTML or Microsoft Office Excel format.



**SEARCHING:** ASTER can be searched by single chemical or multiple chemicals (up to 25).

- Single chemical searching by:
  - CAS Number
  - Chemical Name
  - SMILES String
- Multiple chemical searching by:
  - Comma separated file (\*.csv) of CAS Number or SMILES Strings

## Chemical properties: Single chemical search

The Chemical Properties screen allows you to modify property information to be used in QSAR estimations and/or to obtain details on how a specific property was obtained. To change the property value, type over the existing value on the screen. This changes the source to "user" and modifies the record for the current session only.

The Property table is divided in four sections:

- Property notes the specific property reported
- Values and Units are the value reported or calculated for the property
- Source indicates "calculated" if the property is estimated using a QSAR or other methods, or "EcoChem" if the reported value is from the literature (stored in the EcoChem database)

Selecting the link in the property column will display the calculation of that property.

## Single Chemical Processing

You must use the exact spelling when searching by Chemical Name. If you do not know the exact chemical name, click the "Browse" button to perform a search.

CAS Number:  [Browse Chemicals](#) [Search](#)

Chem Name:  [View Structure](#)

SMILES string:  [Clear Form](#)


CAS Number: 50000 [New Search](#)

Chemical Name: Formaldehyde [Back](#)

[Change](#) [Clear Form](#)

SMILES string: O=C

Chemical Formula: CH2O



Property	Value	Units	Source	Method/Error
Molecular Weight	30.03	g/mole	Calculated	
Parachor	76.20		Calculated	????
Molar Refraction	6.83		Calculated	Av. % Error = 5
Molecular Volume	35.00	cm <sup>3</sup> /g	Calculated	????
LogP (CLogP)	Discontinued July 2011		CLogP	NA
LogP (KowWin)	0.35		KowWin	KowWin v1.67
Melting Point	-92.00	C	EcoChem	
Boiling Point	-21.00	C @ 760 mmHg	EcoChem	
Vapor Pressure		mmHg	Calculated	
Heat of Vaporization	5.39E03	cal/mole	Calculated	Av. % Error = 1.85
Solubility in Water		moles/L	Calculated	
pKa			Calculated	
FH TMOA	10	MOA Number	EcoChem	Carbonyl reactivity (aldehyde eq. #3)

**REPORT SELECTIONS:** Data encoded into ECOTOX undergo a filter process where data meeting minimum test requirements (which are mean values for each species/effect combination and derived from standard test methodologies) are presented along with any data previously evaluated by EPA (e.g., data used in Water Quality Criteria documents). Report options include:

Single Chemical Report (Format: HTML for Profile; Excel for all)

- Profile Report: Chemical, physical/chemical property, and data meeting initial filter requirements
- Supplemental Data Report: Data meeting filter requirement, not median values
- Other Data: ECOTOX data not meeting filter requirements

Multiple Chemical Report (Excel format) - Single row containing chemical identification, and chemical/physical property information, including acute mode of action (MOA), data meeting initial filter requirements and QSARs for four fish species, and one invertebrate species (if model is available for the selected MOA).

Select Report Format:
☒ Profile Report (Geometric Mean, Acute, Chronic and Bioconcentration data)
☐ Supplemental Data Report
☐ Other Data Report

Select Output Format:
☒ HTML (Only available for Profile Report)
☐ MS-Excel

Go

#### I. CHEMICAL IDENTIFICATION

Parameter	Value
Name	Formaldehyde
CAS Number	50000
SMILES	O=C
Formula	CH2O

#### II. ENVIRONMENTAL EXPOSURE ASSESSMENT

Parameter	Value	Source	Reference
Molecular Weight (g/mole)	30.03	Calculated	
Melting Point (C)	-92	EcoChem	
Boiling Point (C)	-21	EcoChem	
Vapor Pressure (mm of Hg)	Not available for this chemical		
Ht Vaporization (cal/mole)	5.39E+03	Calculated	
Solubility in Water (mg/L)	Not available for this chemical		
ClogP	Discontinued July 2015		
KowWin	0.35	KowWin	83336
pKa	Not available for this chemical		
Adsorption Coef (log Koc)	LogP value required		
m**3/mole)	Not available for this chemical		
m**3/mole)	Not available for this chemical		
Hydrolysis Half-life (days)	Hydrolysis unlikely		
BioDegradation Data	Biodegrades Fast Non-Linear Model Prediction: Biodegrades Fast Timeframe: Weeks Timeframe: Days MITI Linear Model Prediction : Readily Degradable Prediction: Readily Degradable <br	BioWin	83338
Mackay Level 1 Environmental Partitioning @ 25C	No value was available for vapour pressure No value was available for aqueous solubility No value was available for log P (log Kow) There is not enough information for the fugacity model		

\*\* Denotes the LogP value used in calculations

#### III. ECOTOXICOLOGICAL HAZARD ASSESSMENT

Table 1. Geometric Means of all data passing the ASTER filter by Species Group

Habitat	Species	Effect	Count	Geo Mean	Min	Max
A	Fish - Acute	MOR	15	38079 ug/L	4960 ug/L	224490 ug/L
A	Fish - Chronic	MOR	1	953900 ug/L	953900 ug/L	953900 ug/L
T	Mammal - Acute	MOR	3	125.98 mg/kg	42 mg/kg	340 mg/kg

Table 2. Median Acute Data values

Habitat	Taxon Group	Name	Int.	Effect	Measure	Media	Dur (d)	Exposure	Median Conc	Source	Ref No
A	Fish	rostrata	LC50	MOR	MORT	FW	4 d	S	83960.00 ug/L	ECOTOX	593
A	Fish	affinis	LC50	MOR	MORT	FW	4 d	S	131300.00 ug/L	ECOTOX	6050
A	Fish	saxatilis	LC50	MOR	MORT	SW	4 d	S	10840.00 ug/L	ECOTOX	3515
A	Fish	promelas	LC50	MOR	MORT	FW	4 d	F	24100.00 ug/L	MED	3217
A	Fish	promelas	LC50	MOR	MORT	FW	4 d	F	24500.00 ug/L	ECOTOX	14339
T	Mammal	musculus	LD50	MOR	MORT	NONE	7 d	IV	42.00 mg/kg	ECOTOX - EDS	104102
T	Mammal	musculus	LD50	MOR	MORT	NONE	7 d	IP	140.00 mg/kg	ECOTOX - EDS	104102
T	Mammal	musculus	LD50	MOR	MORT	NONE	7 d	DT	340.00 mg/kg	ECOTOX - EDS	104102

#### Profile and Multiple Chemical Outputs Include:

- CAS Registry Number
- Chemical Name
- SMILES String
- Molecular Weight
- Melting Point
- Boiling Point
- Vapor Pressure
- Heat of Vaporization
- Solubility in Water
- pKa
- Adsorption Coefficient
- Henry's Constant
- Hydrolysis Half-life
- Biodegradation
- Fugacity
- LogP
- Acute Toxic Mode of Action (MOA)
- ECOTOX Data meeting filter requirements
- Estimated Acute or Chronic Values
- Reference Number
- Full Citation (Profile report only)
- Range of toxicity by taxonomic group (Multiple chemical output only)

**ACCESS:** ASTER is available to EPA employees and contractors via EPA's intranet server (<http://q2626xmnay001.aa.ad.epa.gov/aster/>). Employees of other government agencies (tribal, local, state, national, international) that require a search of the ASTER system must request a search through the GLTED Scientific Outreach staff (E-mail: [ecotox.support@epa.gov](mailto:ecotox.support@epa.gov); T: 218-529-5225), providing SMILES string(s) and/or CAS Registry Number(s) for chemical(s) of interest. Persons affiliated with government contracts/extramural agreements must submit their search requests through the funding governmental agency's Project Officer.

For more information on ASTER: **Telephone:** 218 529 5225 **E mail:** [ecotox.support@epa.gov](mailto:ecotox.support@epa.gov)