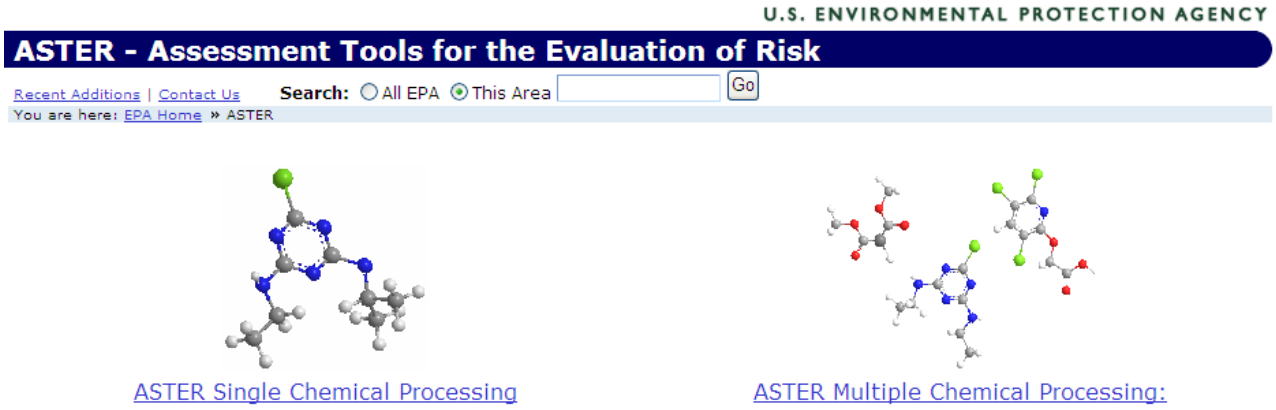
ASTER - Assessment Tools for the Evaluation of Risk

United States Environmental Protection Agency

Information: http://www.epa.gov/med/prods_pubs.htm
Access: http://cfint.rtpnc.epa.gov/aster/

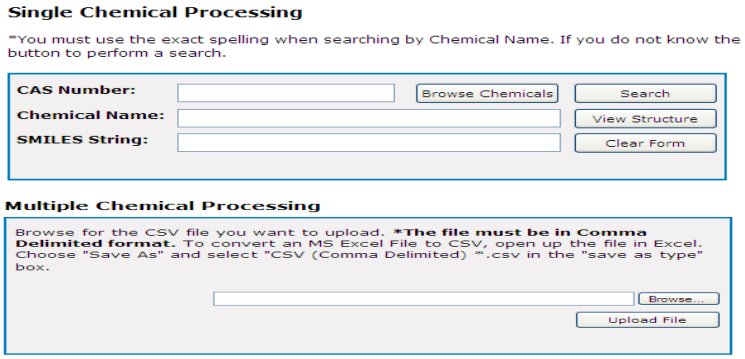


OVERVIEW: ASTER (ASsessment Tools for the Evaluation of Risk) was developed at the U.S. EPA, National Health and Environmental Effects Research Laboratory (NHEERL), Mid-Continent Ecology Division (MED), with funding from the U.S. EPA Office of Solid Waste and Emergency Response, and Office of Research and Development's, National Center for Computational Toxicology. The objective was to develop an intranet application that could assist EPA in hazard ranking and 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 and EcoChem), and QSAR-based estimates when data are lacking.

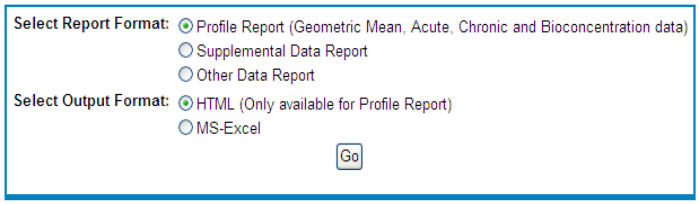
ASTER queries require users to enter a Chemical Abstract Services (CAS) Registry number, a chemical name, or the chemical's structure as represented by a SMILES string. The software allows you to see details on how parameters were calculated or change critical information such as physical/chemical property 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 by multiple chemicals (up to 25).

- Single chemical searching
  - CAS Number
  - Chemical Name
  - SMILES String
- Multiple chemical searching
  - Comma Separated Value (*.csv) file of CAS Numbers or SMILES Strings



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



- Single Chemical Reports (Format: HTML for Profile; Excel for all)
  - Profile Report : contains chemical, physical/chemical property, and data meeting initial filter requirements
  - Supplemental Data Report : data that met filter requirements, which are 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 a model is available for the selected MOA.

For more information on ASTER: **Telephone:** 218 529 5225 **E mail:** ecotox.support@epa.gov

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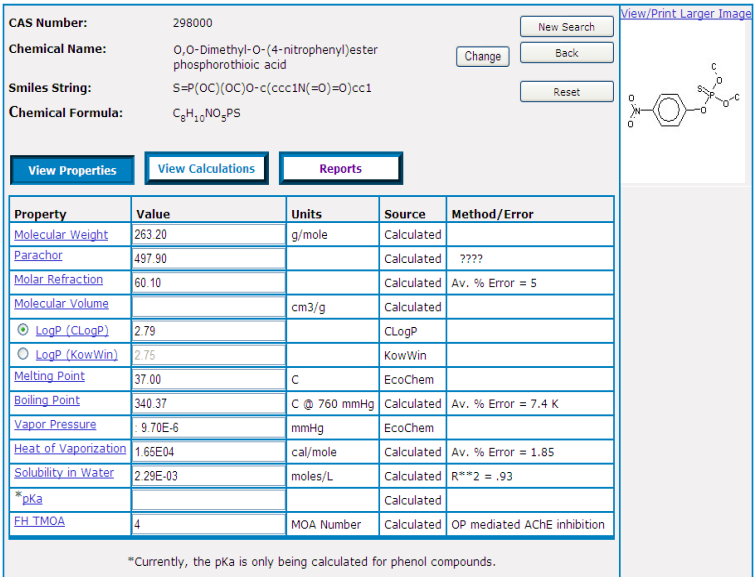
Chemical Properties Screen (Single chemical search): The Chemical Properties screen allows you to modify property information that may be used in QSAR estimations and/or to obtain details on how a certain property was obtained. To change the property value, type over the existing value in the property screen. This changes the source to “User” and only modifies the record for the current session.

The Property table is divided into four sections: Property notes the specific property reported. Value and Units are the value reported or calculated for the property. The Source column will have ”Calculated” if the property is estimated using a QSAR or other method, or ”EcoChem” if the reported value is from the literature and has been stored in the EcoChem database. Selecting the link in the Property column will display the calculation of that property.



CAS Number: 298000
Chemical Name: O,O-Dimethyl-O-(4-nitrophenyl)ester phosphorothioic acid
Smiles String: S=P(OC)(OC)O-c(ccc1N(=O)=O)cc1
Chemical Formula: $C_8H_{10}NO_5PS$

New Search | Back | Change | Reset | View/Print Larger Image

View Properties | View Calculations | Reports

Property	Value	Units	Source	Method/Error
Molecular Weight	263.20	g/mole	Calculated	
Parachor	497.90		Calculated	????
Molar Refraction	60.10		Calculated	Av. % Error = 5
Molecular Volume		cm3/g	Calculated	
LogP (CLogP)	2.79		CLogP	
LogP (KowWin)	2.75		KowWin	
Melting Point	37.00	C	EcoChem	
Boiling Point	340.37	C @ 760 mmHg	Calculated	Av. % Error = 7.4 K
Vapor Pressure	9.70E-6	mmHg	EcoChem	
Heat of Vaporization	1.65E04	cal/mole	Calculated	Av. % Error = 1.85
Solubility in Water	2.29E-03	moles/L	Calculated	R**2 = .93
*pKa			Calculated	
FH TMOA	4	MOA Number	Calculated	OP mediated AChE inhibition

*Currently, the pKa is only being calculated for phenol compounds.

I. CHEMICAL IDENTIFICATION

Parameter	Value
Name	O,O-Dimethyl-O-(4-nitrophenyl)ester phosphorothioic acid
CAS Number	298000
SMILES	S=P(OC)(OC)O-c(ccc1N(=O)=O)cc1
Formula	$C_8H_{10}NO_5PS$

II. ENVIRONMENTAL EXPOSURE ASSESSMENT

Parameter	Value	Source	Reference
Molecular Weight (g/mole)	263.20	Calculated	
Melting Point (C)	37.00	EcoChem	
Boiling Point (C)	340.37	Calculated	
Vapor Pressure (mm of Hg)	Not available for this chemical		
Ht Vaporization (cal/mole)	1.65E04	Calculated	
Solubility in Water (mg/L)	603.80	Calculated	
CLogP	2.79**	CLogP	83337
KowWin	2.75	KowWin	83336
pKa	Not available for this chemical		
Adsorption Coef (log Koc)	2.85	Calculated	
Henry's Constant (atm-m**3/mole)	Not available for this chemical		
Log10 (Henry's Constant)(atm-m**3/mole)	Not available for this chemical		
Hydrolysis Half-life (days)	Not available for this chemical		
BioDegradation Data	Linear Model Prediction : Biodegrades Fast Non-Linear Model Prediction: Biodegrades Fast Ultimate Biodegradation Timeframe: Weeks-Months Primary Biodegradation Timeframe: Days MITI Linear Model Prediction : Not Readily Degradable MITI Non-Linear Model Prediction: Not Readily Degradable	BioWin	83338
Mackay Level 1 Environmental Partitioning @ 25C	No value was available for vapour pressure 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

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 their contractors via EPA’s intranet server (**http://cfint.rtpnc.epa.gov/aster/)** or remotely through Aventail AAA access (https://shield.epa.gov/cfint/aster/). Employees of other government (tribal, local, state, national, international) agencies that require a search of the ASTER system must request a search through the MED Scientific Outreach staff (E-mail: 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.

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