Atrazine

Other names:

1,3,5-Triazine-2,4-diamine, 6-chloro-N-ethyl-N'-(1-methylethyl)-
1,3,5-Triazine-2,4-diamine, 6-chloro-N2-ethyl-N4-(1-methylethyl)-
1-Chloro-3-(ethylamino)-5-(isopropylamino)-2,4,6-triazine
1-Chloro-3-(ethylamino)-5-(isopropylamino)-s-triazine
2-Aethylamino-4-chlor-6-isopropylamino-1,3,5-triazin
2-Chloro-4-(2-propylamino)-6-(ethylamino)-s-triazine
2-Chloro-4-(ethylamino)-6-(isopropylamino)-1,3,5-triazine
2-Chloro-4-(ethylamino)-6-(isopropylamino)-s-triazine
2-Chloro-4-ethylamineisopropylamine-s-triazine
2-Ethylamino-4-isopropylamino-6-chloro-s-triazine
2-chloro-4-(ethylamino)-6-(isopropylamino)triazine
2-chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine
2-chloro-4-ethylamino-6-isopropylamino-s-triazine
6-Chloro-4-(ethylamino)-2-(isopropylamino)-s-triazine
6-Chloro-N-ethyl-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine
6-chloro-N'-ethyl-N-propan-2-yl-1,3,5-triazine-2,4-diamine
A 361
ATZ
Aatram
Aatrex
Aatrex 4L
Aatrex 4LC
Aatrex 80W
Aatrex nine-O
Actinite PK
Akticon
Aktikon
Aktikon PK
Aktinit A
Aktinit PK
Argezin
Atazinax
Atraflow
Atraflow plus
Atranex
Atrasine
Atrataf
Atratol
Atratol A
Atrazin

Atrazine 4L
Atrazine 80W
Atred
Atrex
Attrex
Azinotox 500
Candex
Cekuzina-T
Chromozin
Crisamina
Crisatrina
Crisazine
Cyazin
Farmco atrazine
Farmozine
Fenamin
Fenamine
Fenatrol
Fogard
G 30027
Geigy 30,027
Gesaprim
Gesaprim 50
Gesoprim
Griffex
Griffex 4l
Herbatoxol
Hungazin
Hungazin PK
Inakor
Laddock
Maizina
Mebazine
Oleogesaprim
Pitezin
Primatol
Primatol A
Primaze
Primoleo
Radazin
Radazin T
Radizin
Radizine

	Strazine
	Triazine A 1294
	Vectal
	Vectal SC
	Weedex A
	Wonuk
	Zeaphos
	Zeapos
	Zeazin
	Zeazine
	Zeopos
	azoprim
	gesamprim
	s-Triazine, 2-chloro-4-(ethylamino)-6-(isopropylamino)-
Inchi:	InChI=1S/C8H14ClN5/c1-4-10-7-12-6(9)13-8(14-7)11-5(2)3/h5H,4H2,1-3H3,(H2,10,11,12
InchiKey:	MXWJVTOOROXGIU-UHFFFAOYSA-N
Formula:	C8H14ClN5
SMILES:	CCNc1nc(Cl)nc(NC(C)C)n1
Mol. weight [g/mol]:	215.68
CAS:	1912-24-9

Physical Properties

Property code	Value	Unit	Source
chs	-5047.20 ± 8.90	kJ/mol	NIST Webbook
hfs	-125.40 ± 9.50	kJ/mol	NIST Webbook
log10ws	-3.80		Aqueous Solubility Prediction Method
log10ws	-3.85		Estimated Solubility Method
log10ws	-3.49		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.777		Crippen Method
mcvol	161.960	ml/mol	McGowan Method
rinpol	1708.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1724.00		NIST Webbook

rinpol	1752.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	294.98		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1726.00		NIST Webbook
ripol	2722.00		NIST Webbook
ripol	2747.00		NIST Webbook
ripol	2722.00		NIST Webbook
ripol	2805.00		NIST Webbook
ripol	2776.00		NIST Webbook
ripol	2776.00		NIST Webbook
tf	450.20 ± 0.20	K	NIST Webbook
tf	447.53	K	Aqueous Solubility Prediction Method
tf	447.00	K	Measurement and Correlation of Solubility of 2-Chloro-4-ethylamino-6-isopropylamino-1,3,5-t in Different Organic Solvents
tf	450.49 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	38.15	kJ/mol	449.70	NIST Webbook
hsubt	114.60	kJ/mol	339.00	NIST Webbook
hsubt	113.80	kJ/mol	363.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.74621e+01
Coeff. B	-7.99802e+03
Temperature range (K), min.	465.69
Temperature range (K), max.	658.24

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1912249&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurement and Correlation of Solubility of 2-Chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine in Different Organic Solvents:	https://www.doi.org/10.1021/je400639m
Aqueous Solubility Prediction Method:	http://opensciencechallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point