Simazine

Other names:

1,3,5-Triazine-2,4-diamine, 6-chloro-N,N'-diethyl-
1,3,5-Triazine-2,4-diamine, 6-chloro-N2,N4-diethyl-
1-Chloro-3,5-bis(ethylamino)-2,4,6-triazine
2,4-Bis(ethylamino)-6-chloro-1,3,5-triazine
2,4-Bis(ethylamino)-6-chloro-s-triazine
2,4-Di(ethylamino)-6-chloro-1,3,5-triazine
2-Chloro-4,6-bis(ethylamino)-1,3,5-triazine
2-Chloro-4,6-bis(ethylamino)-s-triazine
2-Chloro-4,6-di(ethylamino)triazine
4,6-Bis(ethylamino)-2-chlorotriazine
6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine
6-Chloro-N,N'-diethyl-[1,3,5]triazin-2,4-diamine
A 2079
Aktinit S
Amizine
Aquazine
Azotop
Batazina
Bitemol
Bitemol S-50
CAT
CAT (herbicide)
CDT
CET
Cekusan
Cekuzina-S
Framed
G 27692
Geigy 27,692
Gesapun
Gesaran
Gesatop
Gesatop 50
H 1803
Herbatoxol S
Herbazin
Herbazin 50
Herbex
Herboxy
Hungazin DT

Premazine
Primatel S
Primatol S
Princep
Printop
Radocon
Radokor
S-Triazine, 2-chloro-4,6-bis(ethylamino)-
Simadex
Simanex
Simatox
Simatsin-neste
Simazin
Simazine 50
Simazine 80W
Symazine
Tafazine
Tafazine 50-W
Taphazine
Triazine A384
W 6658
Yrodazin
Zeapur
s-Triazine, 2,4-bis(ethylamino)-6-chloro-

Inchi: InChI=1S/C7H12ClN5/c1-3-9-6-11-5(8)12-7(13-6)10-4-2/h3-4H2,1-2H3,(H2,9,10,11,12,1

InchiKey: ODCWYMIRDDJXKW-UHFFFAOYSA-N

Formula: C7H12ClN5

SMILES: CCNc1nc(Cl)nc(NCC)n1

Mol. weight [g/mol]: 201.66

CAS: 122-34-9

Physical Properties

Property code	Value	Unit	Source
chs	-4403.70 ± 3.50	kJ/mol	NIST Webbook
hfs	-89.60 ± 4.10	kJ/mol	NIST Webbook
log10ws	-4.55		Estimated Solubility Method
log10ws	-4.55		Aqueous Solubility Prediction Method
logp	1.389		Crippen Method

mcvol	147.870	ml/mol	McGowan Method
rinpol	1704.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1751.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	293.57		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1722.00		NIST Webbook
rinpol	1749.00		NIST Webbook
ripol	2872.00		NIST Webbook
ripol	2806.00		NIST Webbook
ripol	2806.00		NIST Webbook
ripol	2834.00		NIST Webbook
ripol	2806.00		NIST Webbook
ripol	2872.00		NIST Webbook
tf	502.93 ± 0.20	K	NIST Webbook
tf	503.80 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	47.35	kJ/mol	502.50	NIST Webbook
hsubt	130.80	kJ/mol	363.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122349&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point