

Desmetryn

Other names:

1,3,5-Triazine-2,4-diamine, N-methyl-N'-(1-methylethyl)-6-(methylthio)-s-Triazine, 2-(isopropylamino)-4-(methylamino)-6-(methylthio)-Desmetryne
G 34360
GS 34360
Norametryne
Semeron
Semeron 25
Semeron 250
Topusyn
2-Isopropylamino-4-methylamino-6-methylthio-1,3,5-triazine
Desmethryn
2-Isopropylamino-4-methylamino-6-methylthio-1,3,5-triazina
2-Isopropylamino-4-methylamino-6-methylmercapto-s-triazine
2-Methylamino-4-methylthio-6-isopropylamino-1,3,5-triazine
Methylmercapto-4-isopropylamino-6-methylamino-s-triazine
2-Methylthio-4-isopropylamino-6-methylamino-s-triazine
2-(Methylthio)-4-(methylamino)-6-(isopropylamino)-s-triazine
Samuron
2-Methylthio-4-methylamino-6-isopropylamine-1,3,5-triazine
Methylamino-4-methylthio-6-isopropylamino-1,3,5-triazine
Methylthio-4-isopropylamino-6-methylamino-s-triazine
N-Methyl-N'-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine
Triazine, 2-(isopropylamino)-4-(methylamino)-6-(methylthio)-2-Methylmercapto-4-methylamino-6-isopropylamino-s-triazine
2-Methylthio-4-methylamino-6-isopropyl-1,3,5-triazine

Inchi: InChI=1S/C8H15N5S/c1-5(2)10-7-11-6(9-3)12-8(13-7)14-4/h5H,1-4H3,(H2,9,10,11,12,13)

InchiKey: HCRWJJJUKUVORR-UHFFFAOYSA-N

Formula: C8H15N5S

SMILES: CNc1nc(NC(C)C)nc(SC)n1

Mol. weight [g/mol]: 213.30

CAS: 1014-69-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method

logp	1.455		Crippen Method
mcvol	166.070	ml/mol	McGowan Method
rinpol	1815.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1848.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1848.00		NIST Webbook
ripol	2868.00		NIST Webbook
ripol	2889.00		NIST Webbook
ripol	2868.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	101.50	kJ/mol	340.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1014693&Units=SI

Legend

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

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