

Prometryn

Other names:

1,3,5-Triazine-2,4-diamine, N,N'-bis(1-methylethyl)-6-(methylthio)-
2,4-Bis(isopropylamino)-6-(methylmercapto)-s-triazine
2,4-Bis(isopropylamino)-6-(methylthio)-1,3,5-triazine
2,4-Bis(isopropylamino)-6-(methylthio)-s-triazine
2-(Methylmercapto)-4,6-bis(isopropylamino)-s-triazine
2-(Methylthio)-4,6-bis(isopropylamino)-s-triazine
A 1114
Caparol
Caparol 80W
G 34161
Gesagard
Gesagard 50
Gesagarde 50 Wp
Mercasin
Mercazin
Merkazin
N,N'-Bis(1-methylethyl)-6-methylthio-1,3,5-triazine-2,4-diamine
NSC 163049
Polisin
Primatol Q
Promepin
Promethryn
Promethryne
Prometrex
Prometrin
Prometryne
S-Triazine, 2,4-bis(isopropylamino)-6-methylmercapto-
Selectin
Selectin 50
Selektin
Sesagard
Uvon

Inchi: InChI=1S/C10H19N5S/c1-6(2)11-8-13-9(12-7(3)4)15-10(14-8)16-5/h6-7H,1-5H3,(H2,11,**InchiKey:** AAEVYOVXGOFMJO-UHFFFAOYSA-N**Formula:** C10H19N5S**SMILES:** CSc1nc(=NC(C)C)[nH]c(=NC(C)C)[nH]1**Mol. weight [g/mol]:** 241.36**CAS:** 7287-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.10		Estimated Solubility Method
log10ws	-4.10		Aqueous Solubility Prediction Method
logp	0.114		Crippen Method
mcvol	194.250	ml/mol	McGowan Method
rinpol	1919.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1883.00		NIST Webbook
ripol	2758.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.52502e+01
Coeff. B	-1.20241e+04
Temperature range (K), min.	481.69
Temperature range (K), max.	603.05

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7287196&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/ci9903071
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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

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