Prometon

Other names:	(l) N-acetylaspartic acid, diethyl ester
	1,3,5-Triazine-2,4-diamine, 6-methoxy-N,N'-bis(1-methylethyl)-
	1,3,5-Triazine-2,4-diamine, 6-methoxy-N2,N4-bis(1-methylethyl)-
	2,4-Bis(isopropylamino)-6-methoxy-s-triazine
	2,6-Diisopropylamino-4-methoxytriazine
	2-Methoxy-4,6-bis(isopropylamino)-1,3,5-triazine
	2-Methoxy-4,6-bis(isopropylamino)-s-triazine
	2-Methoxy-4,6-bis(isopropylamino)triazine
	4,6-Bis(isopropylamino)-2-methoxy-s-triazine
	G-31435
	Gesafram
	Gesafram 50
	Methoxypropazine
	N,N'-Diisopropyl-6-methoxy-1,3,5-triazine-2,4-diyldiamine
	NSC 163048
	Ontracic 800
	Ontrack
	Ontrack-we-2
	Pramitol
	Pramitol 5P
	Primatol 25e
	Prometone
	s-Triazine, 2,4-bis(isopropylamino)-6-methoxy-
Inchi:	InChI=1S/C10H19N5O/c1-6(2)11-8-13-9(12-7(3)4)15-10(14-8)16-5/h6-7H,1-5H3,(H2,11,
InchiKey:	ISEUFVQQFVOBCY-UHFFFAOYSA-N
Formula:	C10H17N5O
SMILES:	COc1nc(NC(C)C)nc(NC(C)C)n1
Mol. weight [g/mol]:	223.27
CAS:	1610-18-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Estimated Solubility Method
log10ws	-2.48		Aqueous Solubility Prediction Method
logp	1.521		Crippen Method

mcvol	183.770	ml/mol	McGowan Method
rinpol	1704.00		NIST Webbook
rinpol	1704.00		NIST Webbook
ripol	2539.00		NIST Webbook
ripol	2570.00		NIST Webbook
ripol	2539.00		NIST Webbook
ripol	2539.00		NIST Webbook
ripol	2539.00		NIST Webbook
tf	364.65	K	Aqueous Solubility Prediction Method
tf	364.35 ± 0.20	K	NIST Webbook
tf	364.60 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	21.18	kJ/mol	363.50	NIST Webbook
hsubt	92.20	kJ/mol	344.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1610180&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

Legend

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