Pyrimithate

Other names:	Diothyl
	ICI 29661
	O,O-Diethyl O-(2-dimethylamino-6-methyl-4-pyrimidinyl) phosphorothioate
	O-(2-Diethylamino-6-methylpyrimidin-4-yl)-O,O-diethyl phosphorothioate
	O-[2-(Dimethylamino)-6-methyl-4-pyrimidinyl] O,O-diethyl thiophosphate
	Phosphorothioic acid, O-[2-(dimethylamino)-6-methyl-4-pyrimidinyl] O,O-diethyl ester
	Pirimithate
	Pyrimital
	Pyrimithate
Inchi:	InChI=1S/C11H20N3O3PS/c1-6-15-18(19,16-7-2)17-10-8-9(3)12-11(13-10)14(4)5/h8H,6
InchiKey:	MLDVVJZNWASRQL-UHFFFAOYSA-N
Formula:	C11H20N3O3PS
SMILES:	CCOP(=S)(OCC)Oc1cc(C)nc(N(C)C)n1
Mol. weight [g/mol]:	305.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Cheméo Relay (1.0)
logp	2.527		Crippen Method
mcvol	226.450	ml/mol	McGowan Method
tf	294.00	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5221498&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point