

4-Methyl-6-trimethylsilyloxy-2-trimethylsilylsulfan

Other names:	Pyrimidine, 2-mercapto-4-hydroxy-6-methyl, TMS
Inchi:	InChI=1S/C11H22N2OSSi2/c1-9-8-10(14-16(2,3)4)13-11(12-9)15-17(5,6)7/h8H,1-7H3
InchiKey:	MJATVCUNXJRUGB-UHFFFAOYSA-N
Formula:	C11H22N2OSSi2
SMILES:	<chem>Cc1cc(O[Si](C)(C)C)nc(S[Si](C)(C)C)n1</chem>
Mol. weight [g/mol]:	286.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.12		Crippen Method
logp	3.926		Crippen Method
rinpol	1562.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1562.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378219&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/122-418-2/4-Methyl-6-trimethylsilyloxy-2-trimethylsilylsulfanyl-pyrimidine.pdf>

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