Pyrimidine, 4-amino-2-mercapto-5-methyl, TMS

Inchi: InChI=1S/C11H23N3SSi2/c1-9-8-12-11(15-17(5,6)7)13-10(9)14-16(2,3)4/h8H,1-7H3,(H,1

InchiKey: QKXXDMQKGKMFSI-UHFFFAOYSA-N

Formula: C11H23N3SSi2

SMILES: Cc1cnc(S[Si](C)(C)C)nc1N[Si](C)(C)C

Mol. weight [g/mol]: 285.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.69e-03		Crippen Method
logp	3.959		Crippen Method
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R386964&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices