Pyrimidine, 2-mercapto-4-hydroxy, TMS

Other names: 2-Thiouracil, TMS
Inchi: InChI=1S/C10H20N2OSSi2/c1-15(2,3)13-9-7-8-11-10(12-9)14-16(4,5)6/h7-8H,1-6H3
InchiKey: CPULVOVSDZNOPC-UHFFFAOYSA-N
Formula: C10H20N2OSSi2
SMILES: C[Si](C)(C)Oc1ccnc(S[Si](C)(C)C)n1
Mol. weight [g/mol]: 272.51

Physical Properties

Property code	Value	Unit	Source
log10ws	0.36		Crippen Method
logp	3.617		Crippen Method
rinpol	1506.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1512.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R93636&Units=SI
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
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.