Purine, 6-hydroxy-8-mercapto, TMS

Inchi: InChI=1S/C11H20N4OSSi2/c1-18(2,3)16-10-8-9(12-7-13-10)15-11(14-8)17-19(4,5)6/h7H
InchiKey: JXFYAEGMQDCXHS-UHFFFAOYSA-N
Formula: C11H20N4OSSi2
SMILES: C[Si](C)(C)Oc1ncnc2nc(S[Si](C)(C)C)[nH]c12
Mol. weight [g/mol]: 312.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.43		Crippen Method
logp	3.012		Crippen Method
rinpol	2164.00		NIST Webbook
rinpol	2164.00		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=R386637&Units=SI

Legend

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