

Purine, 6-hydroxy-2-mercapto, TMS

Inchi: InChI=1S/C11H20N4OSSi2/c1-18(2,3)16-10-8-9(13-7-12-8)14-11(15-10)17-19(4,5)6/h7H
InchiKey: VHHHGYLNNMMNKBZ-UHFFFAOYSA-N
Formula: C11H20N4OSSi2
SMILES: C[Si](C)(C)Oc1nc(S[Si](C)(C)C)nc2nc[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	2214.00		NIST Webbook
rinpol	2214.00		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=R386593&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/124-547-7/Purine-6-hydroxy-2-mercapto-TMS.pdf>

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