

6-Thioguanine, TMS

Inchi: InChI=1S/C11H21N5OSSi2/c1-19(2,3)16-10-13-8-7(12-11(18)14-8)9(15-10)17-20(4,5)6/
InchiKey: XMTOEIGXUMSAPN-UHFFFAOYSA-N
Formula: C11H21N5OSSi2
SMILES: C[Si](C)(C)Nc1nc(O[Si](C)(C)C)c2[nH]c(=S)[nH]c2n1
Mol. weight [g/mol]: 327.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.67e-03		Crippen Method
logp	2.512		Crippen Method
rinpol	2352.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R93971&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.cheméo.com/cid/53-167-8/6-Thioguanine-TMS.pdf>

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