

2,6-Dithioxanthine, TMS

Inchi: InChI=1S/C14H28N4S2Si3/c1-21(2,3)18-10-15-11-12(18)16-14(20-23(7,8)9)17-13(11)19
InchiKey: BBSYSBBFKXXYEC-UHFFFAOYSA-N
Formula: C14H28N4S2Si3
SMILES: C[Si](C)(C)Sc1nc(S[Si](C)(C)C)c2ncn([Si](C)(C)C)c2n1
Mol. weight [g/mol]: 400.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.17		Crippen Method
logp	5.363		Crippen Method
rinpol	2463.00		NIST Webbook
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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=R93565&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/57-953-1/2-6-Dithioxanthine-TMS.pdf>

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