

Purine, 6-amino-8-mercapto, TMS

Inchi: InChI=1S/C11H21N5SSi2/c1-18(2,3)16-10-8-9(12-7-13-10)15-11(14-8)17-19(4,5)6/h7H,1
InchiKey: OVNCUUABIXTIBA-UHFFFAOYSA-N
Formula: C11H21N5SSi2
SMILES: C[Si](C)(C)Nc1ncnc2nc(S[Si](C)(C)C)[nH]c12
Mol. weight [g/mol]: 311.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.32		Crippen Method
logp	3.045		Crippen Method
rinpol	2301.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R386568&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

Latest version available from:

<https://www.chemeo.com/cid/120-207-8/Purine-6-amino-8-mercapto-TMS.pdf>

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