

2-Hydroxypurine, TMS

Inchi: InChI=1S/C11H20N4OSi2/c1-17(2,3)15-8-13-10-9(15)7-12-11(14-10)16-18(4,5)6/h7-8H,
InchiKey: KWVWRFJQXZJTGG-UHFFFAOYSA-N
Formula: C11H20N4OSi2
SMILES: C[Si](C)(C)Oc1ncc2c(ncn2[Si](C)(C)C)n1
Mol. weight [g/mol]: 280.47

Physical Properties

Property code	Value	Unit	Source
log10ws	0.08		Crippen Method
logp	2.723		Crippen Method
rinpol	1770.00		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=R93583&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/11-968-5/2-Hydroxypurine-TMS.pdf>

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