

2-Hydroxy-6-methylpurine, TMS

Inchi: InChI=1S/C9H14N4OSi/c1-13-6-11-8-7(13)5-10-9(12-8)14-15(2,3)4/h5-6H,1-4H3
InchiKey: SDRCOGBGWONPFE-UHFFFAOYSA-N
Formula: C9H14N4OSi
SMILES: Cn1cnc2nc(O[Si](C)(C)C)ncc21
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	1.577		Crippen Method
rinpol	1784.00		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=R93579&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/56-364-6/2-Hydroxy-6-methylpurine-TMS.pdf>

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