

Purine-8-propanoic acid, 6-hydroxy, TMS

Inchi: InChI=1S/C14H24N4O3Si2/c1-22(2,3)20-11(19)8-7-10-17-12-13(18-10)15-9-16-14(12)21
InchiKey: OVMDUPCQDDAEKM-UHFFFAOYSA-N
Formula: C14H24N4O3Si2
SMILES: C[Si](C)(C)OC(=O)CCc1nc2ncnc(O[Si](C)(C)C)c2[nH]1
Mol. weight [g/mol]: 352.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.19		Crippen Method
logp	2.395		Crippen Method
rinpol	2298.00		NIST Webbook
rinpol	2298.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R386677&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/122-990-7/Purine-8-propanoic-acid-6-hydroxy-TMS.pdf>

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