

Purine, 6-hydroxy-8-hydroxymethyl, TMS

Inchi: InChI=1S/C12H22N4O2Si2/c1-19(2,3)17-7-9-15-10-11(16-9)13-8-14-12(10)18-20(4,5)6/H
InchiKey: FHIPSZYMNMPJFJ-UHFFFAOYSA-N
Formula: C12H22N4O2Si2
SMILES: C[Si](C)(C)OCc1nc2ncnc(O[Si](C)(C)C)c2[nH]1
Mol. weight [g/mol]: 310.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.07		Crippen Method
logp	2.436		Crippen Method
rinpol	1994.00		NIST Webbook
rinpol	1994.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R386622&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/24-202-0/Purine-6-hydroxy-8-hydroxymethyl-TMS.pdf>

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