

Purine, 6-hydroxy-2-methyl, TMS

Inchi: InChI=1S/C9H14N4OSi/c1-6-12-8-7(10-5-11-8)9(13-6)14-15(2,3)4/h5H,1-4H3,(H,10,11,12)H3
InchiKey: XQTSDEGHADWYBU-UHFFFAOYSA-N
Formula: C9H14N4OSi
SMILES: Cc1nc(O[Si](C)(C)C)c2[nH]cnc2n1
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.28		Crippen Method
logp	1.393		Crippen Method
rinpol	1838.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R386602&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/33-438-9/Purine-6-hydroxy-2-methyl-TMS.pdf>

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