

Pyrimidine, 4-hydroxy-6-amino-5-hydroxyacetamino, TMS

Inchi: InChI=1S/C14H30N4O3Si3/c1-22(2,3)18-12-11(17-14(19)21-24(7,8)9)13(16-10-15-12)20
InchiKey: OSFARNFAJOIHOA-UHFFFAOYSA-N
Formula: C14H30N4O3Si3
SMILES: C[Si](C)(C)Nc1ncnc(O[Si](C)(C)C)c1N=C(O)O[Si](C)(C)C
Mol. weight [g/mol]: 386.67

Physical Properties

Property code	Value	Unit	Source
log10ws	2.23		Crippen Method
logp	4.334		Crippen Method
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R386984&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/74-164-8/Pyrimidine-4-hydroxy-6-amino-5-hydroxyacetamino-TMS.pdf>

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