

Pyrimidine, 2,4,6-trihydroxy-5-amino, TMS

Inchi: InChI=1S/C16H37N3O3Si4/c1-23(2,3)19-13-14(20-24(4,5)6)17-16(22-26(10,11)12)18-15
InchiKey: XMSQBRWIJJWAB-UHFFFAOYSA-N
Formula: C16H37N3O3Si4
SMILES: C[Si](C)(C)Nc1c(O[Si](C)(C)C)nc(O[Si](C)(C)C)nc1O[Si](C)(C)C
Mol. weight [g/mol]: 431.83

Physical Properties

Property code	Value	Unit	Source
log10ws	3.08		Crippen Method
logp	5.364		Crippen Method
rinpol	1834.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R386711&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/17-881-5/Pyrimidine-2-4-6-trihydroxy-5-amino-TMS.pdf>

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