

4-Pyrimidinecarboxylic acid, 2,6-bis(trimethylsiloxy)-, trimethylsilyl ester

Other names:

Orotic acid (3TMS)
Orotic acid, tri-TMS
Trimethylsilyl 2,6-bis[(trimethylsilyl)oxy]-4-pyrimidinecarboxylate
Pyrimidin-6-carboxylic acid, 2,4-dihydroxy, tris-TMS
Orotic acid, TMS
Pyrimidin-6-carboxylic acid, 2,4-dihydroxy, TMS
Orotic acid, 3tms derivative

Inchi: InChI=1S/C14H28N2O4Si3/c1-21(2,3)18-12-10-11(13(17)19-22(4,5)6)15-14(16-12)20-23

InchiKey: QOXWEKWDMOZSFV-UHFFFAOYSA-N

Formula: C14H28N2O4Si3

SMILES: C[Si](C)(C)OC(=O)c1cc(O[Si](C)(C)C)nc(O[Si](C)(C)C)n1

Mol. weight [g/mol]: 372.64

CAS: 31111-36-1

Physical Properties

Property code	Value	Unit	Source
log10ws	1.85		Crippen Method
logp	3.896		Crippen Method
rinpol	1749.00		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1752.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C31111361&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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