

Pyrimidine, 2,4-bis[(trimethylsilyl)oxy]-5-[[[(trimethylsilyl)oxy]methyl]methyl]-

Other names:

Pyrimidine, 2,4-bis(trimethylsiloxy)-5-[(trimethylsiloxy)methyl]-
2,4-Bis[(trimethylsilyl)oxy]-5-[[[(trimethylsilyl)oxy]methyl]methyl]pyrimidine
5-Hydroxymethyluracil, tris-TMS
5-Hydroxymethyluracil, TMS
Pyrimidine, 2,4-dihydroxy-5-hydroxymethyl, TMS
5-Hydroxymethyluracil, 3tms derivative

Inchi: InChI=1S/C14H30N2O3Si3/c1-20(2,3)17-11-12-10-15-14(19-22(7,8)9)16-13(12)18-21(4,5)23

InchiKey: WLZGOJADQDKHBW-UHFFFAOYSA-N

Formula: C14H30N2O3Si3

SMILES: C[Si](C)(C)OCc1cnc(O[Si](C)(C)C)nc1O[Si](C)(C)C

Mol. weight [g/mol]: 358.66

CAS: 31517-04-1

Physical Properties

Property code	Value	Unit	Source
log10ws	1.71		Crippen Method
logp	4.255		Crippen Method
rinpol	1673.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1674.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C31517041&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

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