

Threarcic acid, TMS

Inchi: InChI=1S/C16H38O6Si4/c1-23(2,3)19-13(15(17)21-25(7,8)9)14(20-24(4,5)6)16(18)22-26
InchiKey: LPQBQHQEJJCWBZ-KBPBESRZSA-N
Formula: C16H38O6Si4
SMILES: C[Si](C)(C)OC(=O)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 438.81

Physical Properties

Property code	Value	Unit	Source
log10ws	5.15		Crippen Method
logp	4.183		Crippen Method
rinpol	1658.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R101961&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/44-354-0/Threarcic-acid-TMS.pdf>

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