

Propanoic acid, 2-methyl-2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: 2,3-Dihydroxy-2-methylpropanoic acid, 3tms derivative

Inchi: InChI=1S/C13H32O4Si3/c1-13(17-20(8,9)10,11-15-18(2,3)4)12(14)16-19(5,6)7/h11H2,1-

InchiKey: WVOZKTFEMFSGRX-UHFFFAOYSA-N

Formula: C13H32O4Si3

SMILES: CC(CO[Si](C)(C)C)(O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 336.65

CAS: 38166-00-6

Physical Properties

Property code	Value	Unit	Source
log10ws	3.43		Crippen Method
logp	3.826		Crippen Method
rinpol	1348.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C38166006&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

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<https://www.chemeo.com/cid/52-523-3/Propanoic-acid-2-methyl-2-3-bis-trimethylsilyl-oxy-trimethylsilyl-ester.pdf>

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