

Butanoic acid, 2,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: 3-Deoxytetronic acid, tris-TMS
3-Deoxytetronic acid, tri-TMS

Inchi: InChI=1S/C13H32O4Si3/c1-18(2,3)15-11-10-12(16-19(4,5)6)13(14)17-20(7,8)9/h12H,10

InchiKey: LVLAUUNRZLEVPB-UHFFFAOYSA-N

Formula: C13H32O4Si3

SMILES: C[Si](C)(C)OCCC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 336.65

CAS: 55191-52-1

Physical Properties

Property code	Value	Unit	Source
log10ws	3.43		Crippen Method
logp	3.826		Crippen Method
rinpol	1432.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1431.00		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=C55191521&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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