

Butanoic acid, 3,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	2-Deoxytetronic acid, tris-TMS 2-Deoxytetronic acid, tri-TMS
Inchi:	InChI=1S/C13H32O4Si3/c1-18(2,3)15-11-12(16-19(4,5)6)10-13(14)17-20(7,8)9/h12H,10
InchiKey:	OQDJJXAACZVZRO-UHFFFAOYSA-N
Formula:	C13H32O4Si3
SMILES:	C[Si](C)(C)OCC(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	336.65
CAS:	55191-53-2

Physical Properties

Property code	Value	Unit	Source
log10ws	3.43		Crippen Method
logp	3.826		Crippen Method
rinpol	1448.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1448.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55191532&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

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