

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

Other names:	Glyceric acid, tris(trimethylsilyl) deriv.
	Trimethylsilyl 2,3-bis[(trimethylsilyl)oxy]propanoate
	Glyceric acid, (3TMS)
	Glyceric acid, tris-TMS
	Glyceric acid, tri-TMS
	Glyceric acid, TMS
	Glycerate, TMS
	Glyceric acid, 3tms derivative
Inchi:	InChI=1S/C12H30O4Si3/c1-17(2,3)14-10-11(15-18(4,5)6)12(13)16-19(7,8)9/h11H,10H2,
InchiKey:	VTLZEKUPFUIGJQ-UHFFFAOYSA-N
Formula:	C12H30O4Si3
SMILES:	C[Si](C)(C)OCC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	322.62
CAS:	38191-87-6

Physical Properties

Property code	Value	Unit	Source
log10ws	3.85		Crippen Method
logp	3.436		Crippen Method
rinpol	1318.40		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1335.70		NIST Webbook
rinpol	1340.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C38191876&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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