

Bis(dimethyl-t-butylsilyl) oxalate

Other names:	Oxalic acid, bis-DMTBS Oxalic acid, bis(tert-butyldimethylsilyl) ester Oxalic acid, diTBDMS Oxalic acid, bis-TBDMS ester Oxalic acid, TBDMS Oxalic acid, DMTBS Bis[tert-butyl(dimethyl)silyl] oxalate Oxalic acid, 2tbdms derivative
Inchi:	InChI=1S/C14H30O4Si2/c1-13(2,3)19(7,8)17-11(15)12(16)18-20(9,10)14(4,5)6/h1-10H3
InchiKey:	GNBGYVQOJXASGG-UHFFFAOYSA-N
Formula:	C14H30O4Si2
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	318.56
CAS:	104255-91-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.49		Crippen Method
logp	4.083		Crippen Method
rinpol	1548.00		NIST Webbook
rinpol	1538.20		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1538.20		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=C104255916&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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