

Propanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester

Other names: Bis(trimethylsilyl) 2-[(trimethylsilyl)oxy]malonate

Tartronic acid, (tris-TMS)-

Hydroxymalonic acid, tri-TMS

Glyceraric (tartronic) acid, TMS

Hydroxymalonic acid, tris-TMS

Tartronic acid, 3tms derivative

Inchi: InChI=1S/C12H28O5Si3/c1-18(2,3)15-10(11(13)16-19(4,5)6)12(14)17-20(7,8)9/h10H,1-9

InchiKey: FVBGDMUSQDIQPK-UHFFFAOYSA-N

Formula: C₁₂H₂₈O₅Si₃

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

Mol. weight [g/mol]: 336.60

CAS: 38165-93-4

Physical Properties

Property code	Value	Unit	Source
log10ws	4.08		Crippen Method
logp	2.963		Crippen Method
rinpol	1407.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1386.00		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=C38165934&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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