

D-(-)-Citramalic acid, O-trimethylsilyl-, bis(trimethylsilyl) ester

Other names: Bis(trimethylsilyl) (2S)-2-methyl-2-[(trimethylsilyl)oxy]succinate

D-(-)-citramalic acid, 3tms derivative

Inchi: InChI=1S/C14H32O5Si3/c1-14(19-22(8,9)10,13(16)18-21(5,6)7)11-12(15)17-20(2,3)4/h1

InchiKey: PQUDIQABDWAPQW-UHFFFAOYSA-N

Formula: C14H32O5Si3

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

Mol. weight [g/mol]: 364.66

Physical Properties

Property code	Value	Unit	Source
log10ws	3.24		Crippen Method
logp	3.743		Crippen Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1461.60		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1463.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333866&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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