

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

Other names:

2-(Trimethylsiloxy)glutaric acid, bis(trimethylsilyl)- ester
«alpha»-Hydroxyglutaric acid (3TMS)
2-Hydroxyglutaric acid, O,O,O-tris(trimethylsilyl) deriv.
2,3-Dideoxypentanic acid, tris-TMS
Pentanedioic acid, 2-[(trimethylsilyl)oxy]-, 1,5-bis(trimethylsilyl) ester
2-Hydroxyglutaric acid, tris-TMS
2-Hydroxyglutaric acid, tri-TMS
«alpha»-Hydroxyglutaric acid (tms)
2,3-Dideoxypentanic acid, TMS
2-Hydroxyglutaric acid, TMS
2-Hydroxyglutarate, TMS

Inchi:

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

InchiKey:

GFDIGKRHNMDEJF-UHFFFAOYSA-N

Formula:

C₁₄H₃₂O₅Si₃

SMILES:

C[Si](C)(C)OC(=O)CCC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

364.66

CAS:

55530-62-6

Physical Properties

Property code	Value	Unit	Source
log10ws	3.24		Crippen Method
logp	3.743		Crippen Method
rinpol	1581.00		NIST Webbook
rinpol	1615.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1588.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530626&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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<https://www.chemeo.com/cid/15-225-5/Pentanedioic-acid-2-trimethylsilyl-oxy-bis-trimethylsilyl-ester.pdf>

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