

Pentanedioic acid, 3-[(tert-butyl dimethylsilyl)oxy]-3-methyl-, bis(tert-butyl dimethylsilyl) ester

Other names:

3-Hydroxy-3-methylglutaric acid, triTBDMS

3-Hydroxy-3-methylglutarate, TBDMS

3-Hydroxy-3-methylglutaric acid, TBDMS

Meglutol, 3tbdms derivative

Inchi: InChI=1S/C24H52O5Si3/c1-21(2,3)30(11,12)27-19(25)17-24(10,29-32(15,16)23(7,8)9)18

InchiKey: JINZCJWKPQVMQZ-UHFFFAOYSA-N

Formula: C24H52O5Si3

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

Mol. weight [g/mol]: 504.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.95		Crippen Method
logp	7.644		Crippen Method
rinpol	2252.00		NIST Webbook
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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=U221781&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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