

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

Other names: 2-Hydroxyglutaric acid, TBDMS
2-Hydroxyglutarate, TBDMS
2-Hydroxyglutaric acid, triTBDMS

Inchi: InChI=1S/C23H50O5Si3/c1-21(2,3)29(10,11)26-18(20(25)28-31(14,15)23(7,8)9)16-17-19

InchiKey: HZEWZIFIXNHNJX-UHFFFAOYSA-N

Formula: C23H50O5Si3

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

Mol. weight [g/mol]: 490.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.53		Crippen Method
logp	7.254		Crippen Method
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
rinpol	2216.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U221778&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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<https://www.chemeo.com/cid/42-874-5/Pentanedioic-acid-2-tert-butyldimethylsilyl-oxy-bis-tert-butyldimethylsilyl-ester>

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