

3-Hydroxyglutaric acid, triTBDMS

Inchi: InChI=1S/C23H50O5Si3/c1-21(2,3)29(10,11)26-18(16-19(24)27-30(12,13)22(4,5)6)17-20
InchiKey: HEAUNLFVZJDZGH-UHFFFAOYSA-N
Formula: C23H50O5Si3
SMILES: CC(C)(C)[Si](C)(C)OC(=O)CC(CC(=O)O[Si](C)(C)C(C)(C)C)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	2214.00		NIST Webbook
rinpol	2214.00		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=R276614&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/62-688-0/3-Hydroxyglutaric-acid-triTBDMS.pdf>

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