

Isocitric acid, tetraTBDMS

Inchi: InChI=1S/C30H64O7Si4/c1-27(2,3)38(13,14)34-23(31)21-22(25(32)36-40(17,18)29(7,8)30(9,10)11-12)33(15,16)35-24(30)26-28(29)37(19,20)25
InchiKey: VTGQOGVLTQSXMO-UHFFFAOYSA-N
Formula: C30H64O7Si4
SMILES: CC(C)(C)[Si](C)(C)OC(=O)CC(C(=O)O[Si](C)(C)C(C)(C)C)C(O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C(=O)O[Si](C)(C)C(C)(C)C(=O)O
Mol. weight [g/mol]: 649.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.13		Crippen Method
logp	9.028		Crippen Method
rinpol	2632.00		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=R276981&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/25-032-8/Isocitric-acid-tetraTBDMS.pdf>

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