2-Ketoadipic acid mo-tbdms

Other names: 2-Ketohexanedioic acid mo-tbdms
Inchi: InChI=1S/C19H39NO5Si2/c1-18(2,3)26(8,9)24-16(21)14-12-13-15(20-23-7)17(22)25-27(
InchiKey: QZUJNZWYYAUSBD-UHFFFAOYSA-N
Formula: C19H39NO5Si2
SMILES: CON=C(CCCC(=O)O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 417.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	5.256		Crippen Method
rinpol	2103.00		NIST Webbook
rinpol	2103.00		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=U332312&Units=SI

Legend

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