3-Hydroxysebacic acid, tri-TMS

Inchi: InChI=1S/C17H38O5Si3/c1-23(2,3)20-15(14-17(19)22-25(7,8)9)12-10-11-13-16(18)21-24
InchiKey: GGRHSVIGEVXSML-UHFFFAOYSA-N
Formula: C17H38O5Si3
SMILES: C[Si](C)(C)OC(=O)CCCCC(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 406.74

Physical Properties

Property code	Value	Unit	Source
log10ws	1.98		Crippen Method
logp	4.913		Crippen Method
rinpol	2087.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2086.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2087.00		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=R51521&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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