

trans-2-Octenedioic acid, TMS

Inchi: InChI=1S/C14H28O4Si2/c1-19(2,3)17-13(15)11-9-7-8-10-12-14(16)18-20(4,5)6/h9,11H,7
InchiKey: QHCWAYVSWZJFGT-PKNCBQFBNSA-N
Formula: C14H28O4Si2
SMILES: C[Si](C)(C)OC(=O)C=CCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 316.54

Physical Properties

Property code	Value	Unit	Source
log10ws	0.64		Crippen Method
logp	3.859		Crippen Method
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R583972&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/17-947-2/trans-2-Octenedioic-acid-TMS.pdf>

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