

cis-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:	QHWCWAYVSWZJFGT-LUAWRHEFSA-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	1680.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R583927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/60-902-3/cis-2-Octenedioic-acid-TMS.pdf>

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