

3,6-Epoxytetradecanedioic acid, diTMS

Inchi: InChI=1S/C20H40O5Si2/c1-26(2,3)24-19(21)13-11-9-7-8-10-12-17-14-15-18(23-17)16-2
InchiKey: FYMRCDADMMVZJE-UHFFFAOYSA-N
Formula: C20H40O5Si2
SMILES: C[Si](C)(C)OC(=O)CCCCCCC1CCC(CC(=O)O[Si](C)(C)C)O1
Mol. weight [g/mol]: 416.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.23		Crippen Method
logp	5.411		Crippen Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R273195&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/95-878-3/3-6-Epoxytetradecanedioic-acid-diTMS.pdf>

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