

cis-2-Hexenedioic acid, TMS

Inchi: InChI=1S/C12H24O4Si2/c1-17(2,3)15-11(13)9-7-8-10-12(14)16-18(4,5)6/h7,9H,8,10H2,1
InchiKey: BVXJLSYCPJDQEM-CLFYSBASSA-N
Formula: C12H24O4Si2
SMILES: C[Si](C)(C)OC(=O)C=CCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 288.49

Physical Properties

Property code	Value	Unit	Source
log10ws	1.47		Crippen Method
logp	3.079		Crippen Method
rinpol	1492.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R583912&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/20-678-7/cis-2-Hexenedioic-acid-TMS.pdf>

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