

Heptanedioic acid, 3-methyl-, bis(trimethylsilyl) ester

Inchi: InChI=1S/C14H30O4Si2/c1-12(11-14(16)18-20(5,6)7)9-8-10-13(15)17-19(2,3)4/h12H,8-10H,9H2
InchiKey: ZZPGMXASVVDLKE-UHFFFAOYSA-N
Formula: C₁₄H₃₀O₄Si₂
SMILES: CC(CCCC(=O)O[Si](C)(C)C)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 318.56

Physical Properties

Property code	Value	Unit	Source
log10ws	0.73		Crippen Method
logp	3.939		Crippen Method
rinpol	1643.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1643.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U153564&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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<https://www.cheméo.com/cid/125-287-5/Heptanedioic-acid-3-methyl-bis-trimethylsilyl-ester.pdf>

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