Hexanoic acid, dimethyl(3,3,3-trifluoropropyl)silyl ester

Inchi: InChI=1S/C11H21F3O2Si/c1-4-5-6-7-10(15)16-17(2,3)9-8-11(12,13)14/h4-9H2,1-3H3

InchiKey: ALMURUGLURZONM-UHFFFAOYSA-N

Formula: C11H21F3O2Si

SMILES: CCCCCC(=O)O[Si](C)(C)CCC(F)(F)F

Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	4.267		Crippen Method
rinpol	1196.00		NIST Webbook
rinpol	1196.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375593&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/60-212-9/Hexanoic-acid-dimethyl-3-3-3-trifluoropropyl-silyl-ester.pdf

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