Hexanoic acid, (3-cyanopropyl)dimethylsilyl ester

Inchi: InChI=1S/C12H23NO2Si/c1-4-5-6-9-12(14)15-16(2,3)11-8-7-10-13/h4-9,11H2,1-3H3
InchiKey: PCSCOUGJWBHRCI-UHFFFAOYSA-N
Formula: C12H23NO2Si
SMILES: CCCCCC(=O)O[Si](C)(C)CCCC#N
Mol. weight [g/mol]: 241.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.63		Crippen Method
logp	3.619		Crippen Method
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375592&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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