2-Hexanol, (3-cyanopropyl)dimethylsilyl ether

Inchi: InChI=1S/C12H25NOSi/c1-5-6-9-12(2)14-15(3,4)11-8-7-10-13/h12H,5-9,11H2,1-4H3

InchiKey: APUCCJFKFVKFND-UHFFFAOYSA-N

Formula: C12H25NOSi

SMILES: CCCCC(C)O[Si](C)(C)CCCC#N

Mol. weight [g/mol]: 227.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	4.091		Crippen Method
rinpol	1464.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375651&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/14-618-0/2-Hexanol-3-cyanopropyl-dimethylsilyl-ether.pdf

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