

cis-5-Dodecenoic acid, (3-cyanopropyl)dimethylsilyl ester

Inchi: InChI=1S/C18H33NO2Si/c1-4-5-6-7-8-9-10-11-12-15-18(20)21-22(2,3)17-14-13-16-19/h
InchiKey: QAZREVMITNNJJY-KTKRTIGZSA-N
Formula: C18H33NO2Si
SMILES: CCCCCC=CCCC(=O)O[Si](C)(C)CCCC#N
Mol. weight [g/mol]: 323.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	5.735		Crippen Method
rinpol	2179.00		NIST Webbook
rinpol	2179.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375596&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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