(.+/-.)-2-Phenylbutyric acid, (3-cyanopropyl)dimethylsilyl ester

Inchi: InChI=1S/C16H23NO2Si/c1-4-15(14-10-6-5-7-11-14)16(18)19-20(2,3)13-9-8-12-17/h5-7,

InchiKey: CQEKKFPOAVTHMV-UHFFFAOYSA-N

Formula: C16H23NO2Si

SMILES: CCC(C(=O)O[Si](C)(C)CCCC#N)c1ccccc1

Mol. weight [g/mol]: 289.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	4.232		Crippen Method
rinpol	1920.00		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=U375608&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices