1-(3-Cyanopropyl)dimethylsilyloxy-4-methoxyben

Inchi: InChI=1S/C13H19NO2Si/c1-15-12-6-8-13(9-7-12)16-17(2,3)11-5-4-10-14/h6-9H,4-5,11H

InchiKey: XYPQMIGUNYYUQU-UHFFFAOYSA-N

Formula: C13H19NO2Si

SMILES: COc1ccc(O[Si](C)(C)CCCC#N)cc1

Mol. weight [g/mol]: 249.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Crippen Method
logp	3.583		Crippen Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307932&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