

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

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/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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<https://www.cheméo.com/cid/115-417-1/1-3-Cyanopropyl-dimethylsilyloxy-4-methoxybenzene.pdf>

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