

5-Chloro-2-nitrobenzyl alcohol, (3-cyanopropyl)dimethylsilyl ether

Inchi: InChI=1S/C13H17ClN2O3Si/c1-20(2,8-4-3-7-15)19-10-11-9-12(14)5-6-13(11)16(17)18/h
InchiKey: ADUAYPUMBXQASY-UHFFFAOYSA-N
Formula: C13H17ClN2O3Si
SMILES: C[Si](C)(CCCC#N)OCc1cc(Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 312.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	4.274		Crippen Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U376126&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/121-775-7/5-Chloro-2-nitrobenzyl-alcohol-3-cyanopropyl-dimethylsilyl-ether.pdf>

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