

3-Methyl-2-nitrobenzyl alcohol, benzyldimethylsilyl ether

Inchi: InChI=1S/C17H21NO3Si/c1-14-8-7-11-16(17(14)18(19)20)12-21-22(2,3)13-15-9-5-4-6-1
InchiKey: WIVUXBWVTUXHHK-UHFFFAOYSA-N
Formula: C17H21NO3Si
SMILES: Cc1cccc(CO[Si](C)(C)Cc2ccccc2)c1[N+](=O)[O-]
Mol. weight [g/mol]: 315.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	4.407		Crippen Method
rinpol	2201.00		NIST Webbook
rinpol	2201.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U376181&Units=SI>

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.chemeo.com/cid/117-870-6/3-Methyl-2-nitrobenzyl-alcohol-benzyldimethylsilyl-ether.pdf>

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