3-Chloro-2-nitrobenzyl alcohol, benzyldimethylsilyl ether

Inchi: InChI=1S/C16H18ClNO3Si/c1-22(2,12-13-7-4-3-5-8-13)21-11-14-9-6-10-15(17)16(14)18
InchiKey: WRPMFZHIEJDPED-UHFFFAOYSA-N
Formula: C16H18ClNO3Si
SMILES: C[Si](C)(Cc1ccccc1)OCc1cccc(Cl)c1[N+](=O)[O-]
Mol. weight [g/mol]: 335.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	4.752		Crippen Method
rinpol	2296.00		NIST Webbook
rinpol	2296.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U376111&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices