

4-Chloro-3-nitrobenzyl alcohol, bromomethyl dimethylsilyl ether

Inchi: InChI=1S/C10H13BrClNO3Si/c1-17(2,7-11)16-6-8-3-4-9(12)10(5-8)13(14)15/h3-5H,6-7H
InchiKey: QZYOCCLXIFUCEH-UHFFFAOYSA-N
Formula: C10H13BrClNO3Si
SMILES: C[Si](C)(CBr)OCc1ccc(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 338.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	3.904		Crippen Method
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U376118&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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