N-{2-(2-Chlorophenyl)-2-[(trimethylsilyl)oxy]ethyl}

Other names: Benzeneethanamine, 2-chloro-N-(1,1-dimethylethyl)-«beta»-[(trimethylsilyl)oxy]-
Tulobuterol, trimethylsilyl ether
Inchi: InChI=1S/C15H26ClNOSi/c1-15(2,3)17-11-14(18-19(4,5)6)12-9-7-8-10-13(12)16/h7-10,1
InchiKey: LHWGSVJPKWMQJJ-UHFFFAOYSA-N
Formula: C15H26ClNOSi
SMILES: CC(C)(C)NCC(O[Si](C)(C)C)c1ccccc1Cl
Mol. weight [g/mol]: 299.91
CAS: 335627-50-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	4.621		Crippen Method
rinpol	1588.50		NIST Webbook
rinpol	1588.50		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C335627504&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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