2-(2-Chlorophenoxy)ethanol, dimethylpentafluorophenylsilyl ether

Inchi: InChI=1S/C16H14ClF5O2Si/c1-25(2,16-14(21)12(19)11(18)13(20)15(16)22)24-8-7-23-10

InchiKey: NPXJZULDLZUNHI-UHFFFAOYSA-N

Formula: C16H14ClF5O2Si

SMILES: C[Si](C)(OCCOc1ccccc1Cl)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 396.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.92		Crippen Method
logp	4.543		Crippen Method
rinpol	2028.00		NIST Webbook
rinpol	2028.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368260&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices