(4-Chloro-3-nitrophenyl)methanol, dimethylpentafluorophenylsilyl ether

Inchi: InChI=1S/C15H11ClF5NO3Si/c1-26(2,15-13(20)11(18)10(17)12(19)14(15)21)25-6-7-3-4-

InchiKey: UMGHVTIKODWJMD-UHFFFAOYSA-N

Formula: C15H11ClF5NO3Si

SMILES: C[Si](C)(OCc1ccc(Cl)c([N+](=O)[O-])c1)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 411.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.91		Crippen Method
logp	4.573		Crippen Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368747&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