2-(3-Nitrophenyl)ethanol, dimethylpentafluorophenylsilyl ether

Inchi: InChI=1S/C16H14F5NO3Si/c1-26(2,16-14(20)12(18)11(17)13(19)15(16)21)25-7-6-9-4-3-

InchiKey: BGPDHBXXRBCQGT-UHFFFAOYSA-N

Formula: C16H14F5NO3Si

SMILES: C[Si](C)(OCCc1cccc([N+](=O)[O-])c1)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 391.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.15		Crippen Method
logp	3.962		Crippen Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368225&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

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