(2-Methyl-3-nitrophenyl)methanol, dimethylpentafluorophenylsilyl ether

Inchi: InChI=1S/C16H14F5NO3Si/c1-8-9(5-4-6-10(8)22(23)24)7-25-26(2,3)16-14(20)12(18)11(

InchiKey: OQTZUQAXRLMBQK-UHFFFAOYSA-N

Formula: C16H14F5NO3Si

SMILES: Cc1c(CO[Si](C)(C)c2c(F)c(F)c(F)c(F)c2F)cccc1[N+](=O)[O-]

Mol. weight [g/mol]: 391.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.70		Crippen Method
logp	4.228		Crippen Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		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=U367951&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices