

2-(2-Nitrophenyl)ethanol, dimethylpentafluorophenylsilyl ether

Inchi:	InChI=1S/C16H14F5NO3Si/c1-26(2,16-14(20)12(18)11(17)13(19)15(16)21)25-8-7-9-5-3
InchiKey:	FZRYTHTWUXXVON-UHFFFAOYSA-N
Formula:	C16H14F5NO3Si
SMILES:	C[Si](C)(OCCc1cccc1[N+](=O)[O-])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	2070.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/66-570-6/2-2-Nitrophenyl-ethanol-dimethylpentafluorophenylsilyl-ether.pdf>

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