

2-(4-Nitrophenoxy)ethanol, dimethylpentafluorophenylsilyl ether

Inchi: InChI=1S/C16H14F5NO4Si/c1-27(2,16-14(20)12(18)11(17)13(19)15(16)21)26-8-7-25-10
InchiKey: MHHA EIJZGJJLBZ-UHFFFAOYSA-N
Formula: C16H14F5NO4Si
SMILES: C[Si](C)(OCCOc1ccc([N+](=O)[O-])cc1)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 407.36

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -7.89 | | Crippen Method |
| logp | 3.798 | | Crippen Method |
| rinpol | 2402.00 | | NIST Webbook |
| rinpol | 2402.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368928&Units=SI>

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/64-416-9/2-4-Nitrophenoxy-ethanol-dimethylpentafluorophenylsilyl-ether.pdf>

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