

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

Inchi: InChI=1S/C16H14F5NO4Si/c1-25-10-6-8(4-5-9(10)22(23)24)7-26-27(2,3)16-14(20)12(18)
InchiKey: SMSQQJSRDVRRHGJ-UHFFFAOYSA-N
Formula: C16H14F5NO4Si
SMILES: COc1cc(CO[Si](C)(C)c2c(F)c(F)c(F)c2F)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 407.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.35		Crippen Method
logp	3.928		Crippen Method
rinpol	2330.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368932&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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<https://www.chemeo.com/cid/69-578-5/3-Methoxy-4-nitrophenyl-methanol-dimethylpentafluorophenylsilyl-ether.pdf>

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