

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

Inchi: InChI=1S/C16H14F5NO3Si/c1-8-6-9(4-5-10(8)22(23)24)7-25-26(2,3)16-14(20)12(18)11(19)21
InchiKey: VTCSAXKTHJFBHB-UHFFFAOYSA-N
Formula: C16H14F5NO3Si
SMILES: Cc1cc(CO[Si](C)(C)c2c(F)c(F)c(F)c2F)ccc1[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	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368218&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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