2-Isopropylphenol, dimethylpentafluorophenylsilyl ether

Inchi: InChI=1S/C17H17F5OSi/c1-9(2)10-7-5-6-8-11(10)23-24(3,4)17-15(21)13(19)12(18)14(20

InchiKey: MFBVEGAWNYGEDL-UHFFFAOYSA-N

Formula: C17H17F5OSi

SMILES: CC(C)c1ccccc1O[Si](C)(C)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 360.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.50		Crippen Method
logp	4.997		Crippen Method
rinpol	1684.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368961&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/45-579-0/2-Isopropylphenol-dimethylpentafluorophenylsilyl-ether.pdf

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