

2,2,3,4,4,4-Hexafluorobutanol, dimethylpentafluorophenylsilyl ether

Inchi: InChI=1S/C12H9F11OSi/c1-25(2,24-3-11(19,20)10(18)12(21,22)23)9-7(16)5(14)4(13)6(14)
InchiKey: QCZBNGGFWYVFHF-UHFFFAOYSA-N
Formula: C12H9F11OSi
SMILES: C[Si](C)(OCC(F)(F)C(F)C(F)(F)F)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 406.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.67		Crippen Method
logp	4.347		Crippen Method
rinpol	1189.00		NIST Webbook
rinpol	1189.00		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=U368916&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/49-848-7/2-2-3-4-4-4-Hexafluorobutanol-dimethylpentafluorophenylsilyl-ether.pdf>

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