

Heptan-3-ol, dimethylpentafluorophenylsilyl ether

Inchi:	InChI=1S/C15H21F5OSi/c1-5-7-8-9(6-2)21-22(3,4)15-13(19)11(17)10(16)12(18)14(15)20
InchiKey:	GFLRLADGBDPFRN-UHFFFAOYSA-N
Formula:	C15H21F5OSi
SMILES:	CCCCC(CC)O[Si](C)(C)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	340.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.09		Crippen Method
logp	4.780		Crippen Method
rinpol	1458.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368768&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/45-904-8/Heptan-3-ol-dimethylpentafluorophenylsilyl-ether.pdf>

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