

3-Octanol DMPFPS

Inchi: InChI=1S/C16H23F5OSi/c1-5-7-8-9-10(6-2)22-23(3,4)16-14(20)12(18)11(17)13(19)15(16)
InchiKey: MOVMRSPQMIPIEH-UHFFFAOYSA-N
Formula: C16H23F5OSi
SMILES: CCCCCC(CC)O[Si](C)(C)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 354.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.51		Crippen Method
logp	5.170		Crippen Method
rinpol	1535.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R102439&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/15-077-0/3-Octanol-DMPFPS.pdf>

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