

Phenol DMPFPS

Other names: Phenol, FP
Pentafluorophenyldimethylsilyloxybenzene

Inchi: InChI=1S/C14H11F5OSi/c1-21(2,20-8-6-4-3-5-7-8)14-12(18)10(16)9(15)11(17)13(14)19

InchiKey: MOEXGEHFQPNSGK-UHFFFAOYSA-N

Formula: C14H11F5OSi

SMILES: C[Si](C)(Oc1ccccc1)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 318.31

CAS: 71338-91-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.31		Crippen Method
logp	3.873		Crippen Method
rinpol	1490.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1490.00		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=C71338915&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/123-407-3/Phenol-DMPFPS.pdf>

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