

Benzoic acid, 2-pentafluoropropionyloxy-, trimethylsilyl ester

Inchi: InChI=1S/C13H13F5O4Si/c1-23(2,3)22-10(19)8-6-4-5-7-9(8)21-11(20)12(14,15)13(16,17)18
InchiKey: XDWBJRDBGXUWRM-UHFFFAOYSA-N
Formula: C13H13F5O4Si
SMILES: C[Si](C)(C)OC(=O)c1ccccc1OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 356.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	3.781		Crippen Method
rinpol	1351.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375212&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/124-355-0/Benzoic-acid-2-pentafluoropropionyloxy-trimethylsilyl-ester.pdf>

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