

Benzoic acid, 2-chloro, trimethylsilyl ester

Inchi: InChI=1S/C10H13ClO2Si/c1-14(2,3)13-10(12)8-6-4-5-7-9(8)11/h4-7H,1-3H3
InchiKey: GVQHXEQPDBJFRA-UHFFFAOYSA-N
Formula: C10H13ClO2Si
SMILES: C[Si](C)(C)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 228.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	3.332		Crippen Method
rinpol	1388.00		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=R100280&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/114-849-3/Benzoic-acid-2-chloro-trimethylsilyl-ester.pdf>

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