

Benzoic acid, 3-chloro-4-hydroxy, bis-TMS

Inchi: InChI=1S/C13H21ClO3Si2/c1-18(2,3)16-12-8-7-10(9-11(12)14)13(15)17-19(4,5)6/h7-9H,
InchiKey: ZAPABOYUGGWODI-UHFFFAOYSA-N
Formula: C13H21ClO3Si2
SMILES: C[Si](C)(C)OC(=O)c1ccc(O[Si](C)(C)C)c(Cl)c1
Mol. weight [g/mol]: 316.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.30		Crippen Method
logp	4.545		Crippen Method
rinpol	1749.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R100324&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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