Benzoic acid, 3-bromo, TMS

Inchi: InChI=1S/C10H13BrO2Si/c1-14(2,3)13-10(12)8-5-4-6-9(11)7-8/h4-7H,1-3H3
InchiKey: JSPVPBIWAWVXDC-UHFFFAOYSA-N
Formula: C10H13BrO2Si
SMILES: C[Si](C)(C)OC(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 273.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	3.441		Crippen Method
rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R65388&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