Benzoic acid, 4-iodo, TMS

Inchi: InChI=1S/C10H13IO2Si/c1-14(2,3)13-10(12)8-4-6-9(11)7-5-8/h4-7H,1-3H3
InchiKey: SXULXJCDUHIXPH-UHFFFAOYSA-N
Formula: C10H13IO2Si
SMILES: C[Si](C)(C)OC(=O)c1ccc(I)cc1
Mol. weight [g/mol]: 320.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	3.283		Crippen Method
rinpol	1591.00		NIST Webbook
rinpol	1591.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R65413&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices