Benzoic acid, 3,4,5-triiodo, TMS

Inchi: InChI=1S/C10H11I3O2Si/c1-16(2,3)15-10(14)6-4-7(11)9(13)8(12)5-6/h4-5H,1-3H3
InchiKey: TUCLDCNUJZLXEC-UHFFFAOYSA-N
Formula: C10H11I3O2Si
SMILES: C[Si](C)(C)OC(=O)c1cc(I)c(I)c(I)c1
Mol. weight [g/mol]: 571.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	4.492		Crippen Method
rinpol	2381.00		NIST Webbook
rinpol	2381.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R65374&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