

Benzoic acid, 4-bromo, TMS

Inchi: InChI=1S/C10H13BrO2Si/c1-14(2,3)13-10(12)8-4-6-9(11)7-5-8/h4-7H,1-3H3
InchiKey: QGZBFRDBCKZODQ-UHFFFAOYSA-N
Formula: C10H13BrO2Si
SMILES: C[Si](C)(C)OC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 273.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	3.441		Crippen Method
rinpol	1479.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1479.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R65409&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/115-846-5/Benzoic-acid-4-bromo-TMS.pdf>

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