Benzoic acid, 3-methoxy-, trimethylsilyl ester

Other names: Benzoic acid, 3-methoxy, TMS
Inchi: InChI=1S/C11H16O3Si/c1-13-10-7-5-6-9(8-10)11(12)14-15(2,3)4/h5-8H,1-4H3
InchiKey: PPUSJGXNIQTKKU-UHFFFAOYSA-N
Formula: C11H16O3Si
SMILES: COc1cccc(C(=O)O[Si](C)(C)C)c1
Mol. weight [g/mol]: 224.33
CAS: 959111-51-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.72		Crippen Method
logp	2.687		Crippen Method
rinpol	1485.00		NIST Webbook
rinpol	1455.00		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=C959111514&Units=SI

Legend

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