Benzoic acid, 3-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: Benzoic acid, m-(trimethylsiloxy)-, trimethylsilyl ester
m-Hydroxybenzoic acid, (TMS)
Benzoic acid, 3-hydroxy, bis-TMS
Silanol, trimethyl-, m-(trimethylsiloxy)benzoate
3-Hydroxybenzoic acid, TMS
Trimethylsilyl 3-[(trimethylsilyl)oxy]benzoate
3-Hydroxybenzoic acid, 2tms derivative

Inchi: InChI=1S/C13H22O3Si2/c1-17(2,3)15-12-9-7-8-11(10-12)13(14)16-18(4,5)6/h7-10H,1-6H

InchiKey: IKNCKDFNLAAQJI-UHFFFAOYSA-N

Formula: C13H22O3Si2

SMILES: C[Si](C)(C)OC(=O)c1cccc(O[Si](C)(C)C)c1

Mol. weight [g/mol]: 282.48

CAS: 3782-84-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.39		Crippen Method
logp	3.892		Crippen Method
rinpol	1561.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1560.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3782841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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