

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

Other names:	Benzoic acid, m-(trimethylsiloxy)-, methyl ester Methyl ester, trimethylsilyl ether of m-Hydroxybenzoic acid Methyl 3-[(trimethylsilyl)oxy]benzoate
Inchi:	InChI=1S/C11H16O3Si/c1-13-11(12)9-6-5-7-10(8-9)14-15(2,3)4/h5-8H,1-4H3
InchiKey:	NEJLFAOQVKBWGF-UHFFFAOYSA-N
Formula:	C11H16O3Si
SMILES:	COC(=O)c1cccc(O[Si](C)(C)C)c1
Mol. weight [g/mol]:	224.33
CAS:	27798-50-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.72		Crippen Method
logp	2.687		Crippen Method
rinpol	1462.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27798501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/16-711-4/Benzoic-acid-3-trimethylsilyl-oxy-methyl-ester.pdf>

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