

Benzoic acid, 3,4-dihydroxy, methyl ester, DTBS

Inchi:	InChI=1S/C16H24O4Si/c1-15(2,3)21(16(4,5)6)19-12-9-8-11(14(17)18-7)10-13(12)20-21/
InchiKey:	URKUFCXHMWYIOY-UHFFFAOYSA-N
Formula:	C16H24O4Si
SMILES:	COC(=O)c1ccc2c(c1)O[Si](C(C)(C)C)(C(C)(C)C)O2
Mol. weight [g/mol]:	308.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	4.287		Crippen Method
rinpol	1795.00		NIST Webbook
rinpol	1795.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41285&Units=SI

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/68-868-4/Benzoic-acid-3-4-dihydroxy-methyl-ester-DTBS.pdf>

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