

Benzoic acid, 2-hydroxy-3-methyl-4-methoxy, DTBS

Inchi:	InChI=1S/C17H26O4Si/c1-11-13(19-8)10-9-12-14(11)20-22(16(2,3)4,17(5,6)7)21-15(12)
InchiKey:	BZUHHCGKFPAUOT-UHFFFAOYSA-N
Formula:	C17H26O4Si
SMILES:	COc1ccc2c(c1C)O[Si](C(C)(C)C)(C(C)(C)C)OC2=O
Mol. weight [g/mol]:	322.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	4.595		Crippen Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41203&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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/54-593-4/Benzoic-acid-2-hydroxy-3-methyl-4-methoxy-DTBS.pdf>

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