

Benzoic acid, 2-hydroxy-3-methyl-6-(1-methylethyl), DTBS

Inchi:	InChI=1S/C19H30O3Si/c1-12(2)14-11-10-13(3)16-15(14)17(20)22-23(21-16,18(4,5)6)19
InchiKey:	QUSQQWKCZPMLCZ-UHFFFAOYSA-N
Formula:	C19H30O3Si
SMILES:	<chem>Cc1ccc(C(C)C)c2c1O[Si](C(C)(C)C)(C(C)(C)C)OC2=O</chem>
Mol. weight [g/mol]:	334.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	5.710		Crippen Method
rinpol	1945.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41217&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/47-938-9/Benzoic-acid-2-hydroxy-3-methyl-6-1-methylethyl-DTBS.pdf>

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