

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

Inchi: InChI=1S/C16H24O4Si/c1-15(2,3)21(16(4,5)6)19-13-10-11(18-7)8-9-12(13)14(17)20-21/
InchiKey: FTWKLPDBLCOODT-UHFFFAOYSA-N
Formula: C16H24O4Si
SMILES: COc1ccc2c(c1)O[Si](C(C)(C)C)(C(C)(C)C)OC2=O
Mol. weight [g/mol]: 308.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	4.287		Crippen Method
rinpol	1965.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R41235&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/69-342-6/Benzoic-acid-2-hydroxy-4-methoxy-DTBS.pdf>

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