

Benzoic acid, 2-hydroxy-3,6-dimethyl, DTBS

Inchi: InChI=1S/C17H26O3Si/c1-11-9-10-12(2)14-13(11)15(18)20-21(19-14,16(3,4)5)17(6,7)8/
InchiKey: UMYUCQMALOGMND-UHFFFAOYSA-N
Formula: C17H26O3Si
SMILES: Cc1ccc(C)c2c1O[Si](C(C)(C)C)(C(C)(C)C)OC2=O
Mol. weight [g/mol]: 306.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	4.895		Crippen Method
rinpol	1865.00		NIST Webbook
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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=R41178&Units=SI>

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/122-825-0/Benzoic-acid-2-hydroxy-3-6-dimethyl-DTBS.pdf>

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