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

Inchi: InChI=1S/C20H32O3Si/c1-13-11-12-14(18(2,3)4)16-15(13)17(21)23-24(22-16,19(5,6)7)2

InchiKey: DJNIMDVZQSILTG-UHFFFAOYSA-N

Formula: C20H32O3Si

SMILES: Cc1ccc(C(C)(C)C)c2c1C(=O)O[Si](C(C)(C)C)(C(C)(C)C)O2

Mol. weight [g/mol]: 348.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	5.884		Crippen Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R41267&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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