

Benzoic acid, 2-hydroxy-3-(2,3-dioxypopyl), methyl ester, DTBS #1

Inchi: InChI=1S/C19H30O5Si/c1-18(2,3)25(19(4,5)6)23-12-14(24-25)11-13-9-8-10-15(16(13)20)
InchiKey: JFTRHZPZIPLBMY-UHFFFAOYSA-N
Formula: C19H30O5Si
SMILES: COC(=O)c1cccc(CC2CO[Si](C(C)(C)C)(C(C)(C)C)O2)c1O
Mol. weight [g/mol]: 366.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	4.179		Crippen Method
rinpol	2295.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R41146&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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