

Benzoic acid, 2-hydroxy, 3-(2,3-dioxypopyl), bis-DTBS

Inchi: InChI=1S/C26H44O5Si2/c1-23(2,3)32(24(4,5)6)28-17-19(29-32)16-18-14-13-15-20-21(10,11)
InchiKey: TVWNOCFXIYYQPX-UHFFFAOYSA-N
Formula: C26H44O5Si2
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC(=O)c2cccc(CC3CO[Si](C(C)(C)C)(C(C)(C)C)O3)c2O1
Mol. weight [g/mol]: 492.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	7.278		Crippen Method
rinpol	2745.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R41132&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/72-143-3/Benzoic-acid-2-hydroxy-3-2-3-dioxypopyl-bis-DTBS.pdf>

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