

Benzoic acid, 2-hydroxy-5-methyl-3-(1,1-dimethylethyl), DTBS

DTBS

InchiKey:

InChI=1S/C20H32O3Si/c1-13-11-14-16(15(12-13)18(2,3)4)22-24(19(5,6)7,20(8,9)10)23-

RNNQAKPTUWSRGS-UHFFFAOYSA-N

Formula:

C20H32O3Si

SMILES:

Cc1cc2c(c(C(C)(C)C)c1)O[Si](C(C)(C)C)(C(C)(C)C)OC2=O

Mol. weight [g/mol]:

348.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	5.884		Crippen Method
rinpol	2110.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R41249&Units=SI>

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.cheméo.com/cid/37-204-4/Benzoic-acid-2-hydroxy-5-methyl-3-1-1-dimethylethyl-DTBS.pdf>

Generated by Cheméo on 2024-04-28 14:33:45.360443198 +0000 UTC m=+16604074.281020510.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.