

Benzeneacetic acid, 2'-hydroxy, DTBS

Inchi: InChI=1S/C16H24O3Si/c1-15(2,3)20(16(4,5)6)18-13-10-8-7-9-12(13)11-14(17)19-20/h7-
InchiKey: SQEGAFIHDXGHL-UHFFFAOYSA-N
Formula: C16H24O3Si
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC(=O)Cc2ccccc2O1
Mol. weight [g/mol]: 292.45

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.71 | | Crippen Method |
| logp | 4.207 | | Crippen Method |
| rinpol | 1845.00 | | NIST Webbook |
| rinpol | 1845.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R41089&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/125-125-4/Benzeneacetic-acid-2-hydroxy-DTBS.pdf>

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