

Benzoic acid, 2-hydroxy-6-methoxy, DTBS

Inchi: InChI=1S/C16H24O4Si/c1-15(2,3)21(16(4,5)6)19-12-10-8-9-11(18-7)13(12)14(17)20-21/
InchiKey: UWTOAAIJMABADM-UHFFFAOYSA-N
Formula: C16H24O4Si
SMILES: COc1cccc2c1C(=O)O[Si](C(C)(C)C)(C(C)(C)C)O2
Mol. weight [g/mol]: 308.44

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.99 | | Crippen Method |
| logp | 4.287 | | Crippen Method |
| rinpol | 1940.00 | | NIST Webbook |
| rinpol | 1940.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R41253&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.chemeo.com/cid/113-994-3/Benzoic-acid-2-hydroxy-6-methoxy-DTBS.pdf>

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