

Guaiacol, tert-butyldimethylsilyl ether

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|-----------------------------|---|
| Other names: | Guaiacol, tbdms derivative |
| Inchi: | InChI=1S/C13H22O2Si/c1-13(2,3)16(5,6)15-12-10-8-7-9-11(12)14-4/h7-10H,1-6H3 |
| InchiKey: | PUOZJZXUPFEFNR-UHFFFAOYSA-N |
| Formula: | C13H22O2Si |
| SMILES: | COc1ccccc1O[Si](C)(C)C(C)(C)C |
| Mol. weight [g/mol]: | 238.40 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.85 | | Crippen Method |
| logp | 4.079 | | Crippen Method |
| rinpol | 1462.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U333460&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/49-178-1/Guaiacol-tert-butyldimethylsilyl-ether.pdf>

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