

3-Hydroxy-4-methoxybenzaldehyde, trimethylsilyl ether

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|----------------------|---|
| Other names: | Isovanillin, tms derivative |
| Inchi: | InChI=1S/C11H16O3Si/c1-13-10-6-5-9(8-12)7-11(10)14-15(2,3)4/h5-8H,1-4H3 |
| InchiKey: | TYQCHITWYOTIFA-UHFFFAOYSA-N |
| Formula: | C11H16O3Si |
| SMILES: | COc1ccc(C=O)cc1O[Si](C)(C)C |
| Mol. weight [g/mol]: | 224.33 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.84 | | Crippen Method |
| logp | 2.721 | | Crippen Method |
| rinpol | 1521.00 | | NIST Webbook |
| rinpol | 1563.10 | | NIST Webbook |
| rinpol | 1521.00 | | NIST Webbook |
| rinpol | 1563.10 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U352851&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/95-127-6/3-Hydroxy-4-methoxybenzaldehyde-trimethylsilyl-ether.pdf>

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