

4'-Hydroxy-3'-methoxyacetophenone, trimethylsilyl ether

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|----------------------|--|
| Other names: | Acetovanillone, tms derivative |
| Inchi: | InChI=1S/C12H18O3Si/c1-9(13)10-6-7-11(12(8-10)14-2)15-16(3,4)5/h6-8H,1-5H3 |
| InchiKey: | MKPNSCQBWMXUEF-UHFFFAOYSA-N |
| Formula: | C12H18O3Si |
| SMILES: | COc1cc(C(C)=O)ccc1O[Si](C)(C)C |
| Mol. weight [g/mol]: | 238.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.26 | | Crippen Method |
| logp | 3.111 | | Crippen Method |
| rinsol | 1626.10 | | NIST Webbook |
| rinsol | 1626.10 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U352842&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| rinsol: | Non-polar retention indices |

Latest version available from:

<https://www.chemeo.com/cid/33-037-4/4-Hydroxy-3-methoxyacetophenone-trimethylsilyl-ether.pdf>

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