

4-Hydroxycoumarin, trimethylsilyl ether

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|-----------------------------|---|
| Other names: | 4-[(Trimethylsilyl)oxy]-2H-chromen-2-one 4-Hydroxycoumarin TMS Coumarin, 4-hydroxy-, TMS 4-Hydroxycoumarin, tms derivative |
| Inchi: | InChI=1S/C12H14O3Si/c1-16(2,3)15-11-8-12(13)14-10-7-5-4-6-9(10)11/h4-8H,1-3H3 |
| InchiKey: | COEQTMDELCKFP-UHFFFAOYSA-N |
| Formula: | C12H14O3Si |
| SMILES: | C[Si](C)(C)Oc1cc(=O)oc2ccccc12 |
| Mol. weight [g/mol]: | 234.32 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -5.44 | | Crippen Method |
| logp | 3.007 | | Crippen Method |
| rinpol | 1863.50 | | NIST Webbook |
| rinpol | 1869.50 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U333104&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|-------------------------------------|
| 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/52-582-8/4-Hydroxycoumarin-trimethylsilyl-ether.pdf>

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