

Eicosanoic acid, 20-hydroxy, methyl ester, TMS

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|-----------------------------|--|
| Other names: | 20-hydroxyeicosanoic acid, methyl ester TMSi ether |
| Inchi: | InChI=1S/C24H50O3Si/c1-26-24(25)22-20-18-16-14-12-10-8-6-5-7-9-11-13-15-17-19-21 |
| InchiKey: | MZIRYUHQXQMARZ-UHFFFAOYSA-N |
| Formula: | C24H50O3Si |
| SMILES: | COC(=O)CCCCCCCCCCCCCCCCCCCCO[Si](C)(C)C |
| Mol. weight [g/mol]: | 414.74 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -5.87 | | Crippen Method |
| logp | 8.033 | | Crippen Method |
| rinpol | 2680.00 | | NIST Webbook |
| rinpol | 2665.00 | | NIST Webbook |
| rinpol | 2680.00 | | NIST Webbook |
| rinpol | 2665.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R383727&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/83-976-7/Eicosanoic-acid-20-hydroxy-methyl-ester-TMS.pdf>

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