

S-Methoxycarbonylcysteine, MTH-TMS

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|-----------------------------|---------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C10H18N2O3S2Si/c1-12-8(15-18(3,4)5)7(11-9(12)16)6-17-10(13)14-2/h6H2,1 |
| InchiKey: | KNUINTXZPGVJDC-UHFFFAOYSA-N |
| Formula: | C10H18N2O3S2Si |
| SMILES: | COC(=O)SCc1[nH]c(=S)n(C)c1O[Si](C)(C)C |
| Mol. weight [g/mol]: | 306.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.28 | | Crippen Method |
| logp | 2.814 | | Crippen Method |
| rinpol | 1546.00 | | NIST Webbook |
| rinpol | 1546.00 | | NIST Webbook |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R525505&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 |
| rinpol: | Non-polar retention indices |

Latest version available from:

<https://www.chemeo.com/cid/42-211-0/S-Methoxycarbonylcysteine-MTH-TMS.pdf>

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