

6-Azathymine, bis(trimethylsilyl) ether

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|-----------------------------|--|
| Other names: | 6-Azathymine, TMS |
| Inchi: | InChI=1S/C10H21N3O2Si2/c1-8-9(14-16(2,3)4)11-10(13-12-8)15-17(5,6)7/h1-7H3 |
| InchiKey: | WFMAXSXEHMITKR-UHFFFAOYSA-N |
| Formula: | C10H21N3O2Si2 |
| SMILES: | Cc1nnc(O[Si](C)(C)C)nc1O[Si](C)(C)C |
| Mol. weight [g/mol]: | 271.46 |
| CAS: | 17331-64-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 0.74 | | Crippen Method |
| logp | 2.607 | | Crippen Method |
| rinpol | 1459.80 | | NIST Webbook |
| rinpol | 1500.00 | | NIST Webbook |
| rinpol | 1500.00 | | NIST Webbook |
| rinpol | 1467.60 | | NIST Webbook |
| rinpol | 1459.80 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C17331645&Units=SI |

Legend

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

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