

6-Azauracil, TMS

Inchi: InChI=1S/C9H19N3O2Si2/c1-15(2,3)13-8-7-10-12-9(11-8)14-16(4,5)6/h7H,1-6H3
InchiKey: MNMOUFWORYTNCL-UHFFFAOYSA-N
Formula: C9H19N3O2Si2
SMILES: C[Si](C)(C)Oc1cnnc(O[Si](C)(C)C)n1
Mol. weight [g/mol]: 257.44

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 1.22 | | Crippen Method |
| logp | 2.299 | | Crippen Method |
| rinpol | 1449.90 | | NIST Webbook |
| rinpol | 1454.00 | | NIST Webbook |
| rinpol | 1449.90 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R5988&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/59-322-9/6-Azauracil-TMS.pdf>

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