

«alpha»-Pseudouridine, TMS

Inchi: InChI=1S/C21H44N2O6Si4/c1-30(2,3)25-15-16-18(28-32(7,8)9)19(29-33(10,11)12)20(26)
InchiKey: GQVVRBIFPVSHCQ-UDLHLFEOSA-N
Formula: C21H44N2O6Si4
SMILES: C[Si](C)(C)OCC1OC(n2ccc(O[Si](C)(C)C)nc2=O)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 532.93

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 3.86 | | Crippen Method |
| logp | 4.646 | | Crippen Method |
| rinpol | 2332.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R134431&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/42-481-1/alpha-Pseudouridine-TMS.pdf>

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