

4-Pyrimidinecarboxylic acid, 2,6-bis[(tert-butyl dimethylsilyl)oxy]-, tert-butyl dimethylsilyl ester

Other names: Orotic acid, bis(tert-butyl dimethylsilyl)-, tert-butyl dimethylsilyl ester
Orotic acid, TBDMS

Inchi: InChI=1S/C23H46N2O4Si3/c1-21(2,3)30(10,11)27-18-16-17(19(26)28-31(12,13)22(4,5)6
InchiKey: KYXHYBLGLQCYAV-UHFFFAOYSA-N
Formula: C23H46N2O4Si3
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cc(O[Si](C)(C)C(C)(C)C)nc(O[Si](C)(C)C(C)(C)C)n1
Mol. weight [g/mol]: 498.88
CAS: 959264-61-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.92 | | Crippen Method |
| logp | 7.407 | | Crippen Method |
| rinpol | 2390.00 | | NIST Webbook |
| rinpol | 2390.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C959264610&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

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