

1,6-Anhydroiditol, TMS

Inchi: InChI=1S/C18H44O5Si4/c1-24(2,3)20-15-13-19-14-16(21-25(4,5)6)18(23-27(10,11)12)17
InchiKey: IKGHVFJGAOMATA-UHFFFAOYSA-N
Formula: C18H44O5Si4
SMILES: C[Si](C)(C)OC1COCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 452.88

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 4.66 | | Crippen Method |
| logp | 4.897 | | Crippen Method |
| rinpol | 1813.00 | | NIST Webbook |
| rinpol | 1813.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R74266&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/125-039-0/1-6-Anhydroiditol-TMS.pdf>

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