

2-Thiobarbituric acid, S-trimethylsilyl-, bis(trimethylsilyl) ether

Inchi: InChI=1S/C13H28N2O2SSi3/c1-19(2,3)16-11-10-12(17-20(4,5)6)15-13(14-11)18-21(7,8)
InchiKey: JHNMKPPCNCDCY-UHFFFAOYSA-N
Formula: C13H28N2O2SSi3
SMILES: C[Si](C)(C)Oc1cc(O[Si](C)(C)C)nc(S[Si](C)(C)C)n1
Mol. weight [g/mol]: 360.69

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 1.35 | | Crippen Method |
| logp | 4.831 | | Crippen Method |
| rinpol | 1781.00 | | NIST Webbook |
| rinpol | 1761.80 | | NIST Webbook |
| rinpol | 1781.00 | | NIST Webbook |
| rinpol | 1761.80 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352469&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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