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: JHNMKCPPCNCDCY-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/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices