3-Methylxanthine, TMS

Inchi: InChI=1S/C12H22N4O2Si2/c1-15-11(17)9-10(14-12(15)18-20(5,6)7)16(8-13-9)19(2,3)4/h
InchiKey: OIMZLKYFVAVESI-UHFFFAOYSA-N
Formula: C12H22N4O2Si2
SMILES: Cn1c(O[Si](C)(C)C)nc2c(ncn2[Si](C)(C)C)c1=O
Mol. weight [g/mol]: 310.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.86		Crippen Method
logp	2.027		Crippen Method
rinpol	1919.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R93707&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices