1-Methylxanthine, TMS

Inchi: InChI=1S/C12H22N4O2Si2/c1-16-10-9(13-8-14-10)11(17-19(2,3)4)15-12(16)18-20(5,6)7
InchiKey: JSOSLNJQDQLTGO-UHFFFAOYSA-N
Formula: C12H22N4O2Si2
SMILES: Cn1c(O[Si](C)(C)C)nc(O[Si](C)(C)C)c2ncnc1-2
Mol. weight [g/mol]: 310.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	2.742		Crippen Method
rinpol	2052.00		NIST Webbook
rinpol	2052.00		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=R93547&Units=SI

Legend

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