7-Methylxanthine, bis(trimethylsilyl) derivative

Other names: 7-Methylxanthine, 2tms derivative
Inchi: InChI=1S/C12H22N4O2Si2/c1-14-8-13-10-9(14)11(17)16(20(5,6)7)12(18)15(10)19(2,3)4
InchiKey: XGBUDYKEDOGSQK-UHFFFAOYSA-N
Formula: C12H22N4O2Si2
SMILES: Cn1cnc2c1c(=O)n([Si](C)(C)C)c(=O)n2[Si](C)(C)C
Mol. weight [g/mol]: 310.50

Physical Properties

Property code	Value	Unit	Source
log10ws	0.15		Crippen Method
logp	1.263		Crippen Method
rinpol	2054.40		NIST Webbook
rinpol	2054.40		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=U333949&Units=SI

Legend

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