

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
rinsol	2054.40		NIST Webbook
rinsol	2054.40		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/113-544-2/7-Methylxanthine-bis-trimethylsilyl-derivative.pdf>

Generated by Cheméo on 2024-05-03 15:53:47.896084016 +0000 UTC m=+17040876.816661331.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.