

1,3-Dimethylxanthine, TMS

Inchi:	InChI=1S/C10H18N4O2Si/c1-12-8-7(9(15)13(2)10(12)16)14(6-11-8)17(3,4)5/h6-8H,1-5H
InchiKey:	CMRKZRQPMRTUOJ-UHFFFAOYSA-N
Formula:	C10H18N4O2Si
SMILES:	CN1C(=O)C2C(N=CN2[Si](C)(C)C)N(C)C1=O
Mol. weight [g/mol]:	254.36

Physical Properties

Property code	Value	Unit	Source
log10ws	1.53		Crippen Method
logp	0.384		Crippen Method
rinpol	1875.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R93444&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/59-969-2/1-3-Dimethylxanthine-TMS.pdf>

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