

1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-(trimethylsilyl)-

Other names:	Theophylline TMS derivative Theophylline, TMS DPT-TMS
Inchi:	InChI=1S/C10H16N4O2Si/c1-12-8-7(9(15)13(2)10(12)16)14(6-11-8)17(3,4)5/h6H,1-5H3
InchiKey:	KPBTTYFAGBODJB-UHFFFAOYSA-N
Formula:	C10H16N4O2Si
SMILES:	Cn1c(=O)c2c(ncn2[Si](C)(C)C)n(C)c1=O
Mol. weight [g/mol]:	252.35
CAS:	62374-32-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	0.117		Crippen Method

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=C62374327&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/119-992-9/1H-Purine-2-6-dione-3-7-dihydro-1-3-dimethyl-7-trimethylsilyl.pdf>

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