

Inosine, tetramethyl ether

Other names:	Inosine, o-tetrakis(trimethylsilyl) ether
Inchi:	InChI=1S/C14H20N4O5/c1-19-5-8-10(20-2)11(21-3)14(23-8)18-7-17-9-12(18)15-6-16-13
InchiKey:	ZJAOTVCRECWWD-UHFFFAOYSA-N
Formula:	C14H20N4O5
SMILES:	COCC1OC(n2cnc3c(OC)ncnc32)C(OC)C1OC
Mol. weight [g/mol]:	324.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	0.409		Crippen Method
mcvol	227.610	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332746&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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