1,3,7,9-Tetramethyluric acid

Other names:	Tetramethyl uric acid
	1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-1,3,7,9-tetramethyl-
	Ba 2750
	Temorine
	Temurin
	Uric acid, 1,3,7,9-tetramethyl-
Inchi:	InChI=1S/C9H12N4O3/c1-10-5-6(11(2)8(10)15)12(3)9(16)13(4)7(5)14/h1-4H3
InchiKey:	QGDOQULISIQFHQ-UHFFFAOYSA-N
Formula:	C9H12N4O3
SMILES:	Cn1c(=O)c2c(n(C)c1=O)n(C)c(=O)n2C
Mol. weight [g/mol]:	224.22
CAS:	2309-49-1

Physical Properties

Property code	Value	Unit	Source
ie	7.91	eV	NIST Webbook
ie	7.90 ± 0.10	eV	NIST Webbook
log10ws	-6.69		Crippen Method
logp	-1.726		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
rinpol	2183.00		NIST Webbook
rinpol	2183.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2309491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices