

Tetramethyluric acid

Other names: 1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-1,3,7,9-tetramethyl-; Ba 2750; Temorine; Temurin; Tetramethyl uric acid; 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

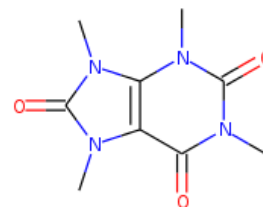
InChI Key: QGDOQULISIQFHQ-UHFFFAOYSA-N

Formula: C₉H₁₂N₄O₃

SMILES: Cn1c2c(n(C)c1=O)n(C)c(=O)n(C)c2=O

Molecular Weight: 224.22

CAS: 2309-49-1



Physical Properties

Property	Value	Unit	Source
IE	7.91	eV	NIST Webbook
IE	7.90 ± 0.10	eV	NIST Webbook
$\log P_{\text{oct/wat}}$	-1.726		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H12N4O3/c1-10-5-6\(11\(2\)8\(10\)15\)12\(3\)9\(16\)13\(4\)7\(5\)14/h1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H12N4O3/c1-10-5-6(11(2)8(10)15)12(3)9(16)13(4)7(5)14/h1-4H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

IE: Ionization energy (eV).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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