1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-1,3,7-trimethyl-

Other names: 1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-1,3,7-trimethyl-
Ba 2753
Uric acid, 1,3,7-trimethyl-
7,9-dihydro-1,3,7-trimethyl-1H-purine-2,6,8(3H)-trione

Inchi: InChI=1S/C8H10N4O3/c1-10-4-5(9-7(10)14)11(2)8(15)12(3)6(4)13/h1-3H3,(H,9,14)

InchiKey: BYXCFUMGEBZDDI-UHFFFAOYSA-N

Formula: C8H10N4O3

SMILES: Cn1c(=O)c2c([nH]c(=O)n2C)n(C)c1=O

Mol. weight [g/mol]: 210.19

Physical Properties

Property code	Value	Unit	Source
ie	7.98	eV	Cheméo Relay (1.0)
logp	-2.218		Crippen Method
mcvol	142.190	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5415441&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

ie: Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume