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

Other names: Uric acid, 1,3-dimethyl-
Ba 2751
Oxytheophylline
1,3-Dimethyluric acid
7,9-dihydro-1,3-dimethyl-1H-purine-2,6,8(3H)-trione

Inchi: InChI=1S/C7H8N4O3/c1-10-4-3(8-6(13)9-4)5(12)11(2)7(10)14/h1-2H3,(H2,8,9,13)

InchiKey: OTSBKHHWSQYEHK-UHFFFAOYSA-N

Formula: C7H8N4O3

SMILES: Cn1c(=O)c2[nH]c(=O)[nH]c2n(C)c1=O

Mol. weight [g/mol]: 196.16

CAS: 944-73-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	-2.710		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
rinpol	2052.00		NIST Webbook
rinpol	2052.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C944730&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices