

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

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