

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

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