Acefylline Piperazine

Other names:	Acepifylline
Inchi:	1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-7H-purine-7-acetic acid, compound with piperazine (2:1) InChI=1S/C9H10N4O4/c1-11-7-6(8(16)12(2)9(11)17)13(4-10-7)3-5(14)15/h4H,3H2,1-2H
InchiKey:	HCYFGRCYSCXKNQ-UHFFFAOYSA-N
Formula:	C9H10N4O4
SMILES:	Cn1c(=O)c2c(ncn2CC(=O)O)n(C)c1=O
Mol. weight [g/mol]:	238.20
CAS:	18833-13-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	-1.482		Crippen Method
mcvol	157.850	ml/mol	McGowan Method
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C18833131&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices