1H-Purine-2,6-dione, 7-ethyl-3,7-dihydro-1,3-dimethyl-

Other names:	7-Ethyl-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione
	7-Ethyl-1,3-dimethylxanthine
	7-Ethyltheophylline
	Ethylteofyllin
	Ethyltheophylline
	NSC 515485
	Theophylline, 7-ethyl-
Inchi:	InChI=1S/C9H12N4O2/c1-4-13-5-10-7-6(13)8(14)12(3)9(15)11(7)2/h5H,4H2,1-3H3
InchiKey:	RPOQNHMXOPWCEK-UHFFFAOYSA-N
Formula:	C9H12N4O2
SMILES:	CCn1cnc2c1c(=O)n(C)c(=O)n2C
Mol. weight [g/mol]:	208.22
CAS:	23043-88-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.76		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.546		Crippen Method
mcvol	150.410	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23043881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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