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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23043881&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume