# 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