

# Theophylline

**Other names:**

1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate  
1H-Purine-2,6-dione, 3,9-dihydro-1,3-dimethyl-, hydrate (1:1)  
theophylline monohydrate

**Inchi:** InChI=1S/C7H8N4O2.H2O/c1-10-5-4(8-3-9-5)6(12)11(2)7(10)13;/h3H,1-2H3,(H,8,9);1H2**InchiKey:** INQSMEFCAIHTJG-UHFFFAOYSA-N**Formula:** C7H10N4O3**SMILES:** Cn1c(=O)c2[nH]cnc2n(C)c1=O.O**Mol. weight [g/mol]:** 198.18**CAS:** 5967-84-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.32		Aqueous Solubility Prediction Method
log10ws	-1.39		Estimated Solubility Method
tf	544.98	K	Aqueous Solubility Prediction Method

## Sources

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5967840&Units=SI>**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

## Legend

**log10ws:** Log10 of Water solubility in mol/l**tf:** Normal melting (fusion) point

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