

# 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(phenylmethyl)-

Other names:

8-Benzyltheophylline

8-benzyl-3,7-dihydro-1,3-dimethyl-1H-purine-2,6-dione

8-(phenylmethyl)theophylline

**Inchi:** InChI=1S/C14H14N4O2/c1-17-12-11(13(19)18(2)14(17)20)15-10(16-12)8-9-6-4-3-5-7-9/

**InchiKey:** SWKGFZTXWQMFLK-UHFFFAOYSA-N

**Formula:** C14H14N4O2

**SMILES:** Cn1c(=O)c2[nH]c(Cc3ccccc3)nc2n(C)c1=O

**Mol. weight [g/mol]:** 270.29

**CAS:** 2879-15-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.78		Crippen Method
logp	0.069		Crippen Method
mcvol	197.100	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2879154&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**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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