

# Etamiphyllin

**Other names:**

1H-Purine-2,6-dione, 7-[2-(diethylamino)ethyl]-3,7-dihydro-1,3-dimethyl-  
Camphophylline  
Corafil  
Diaethylaminoethyl-theophyllin  
Diethylaminoethyltheophylline  
Etaminophylline  
Etamiphylline  
Milliphylline  
Millophylline  
Parephyllin  
Queryl  
R-3588  
Solufilina  
Soluphylline  
Theophylline, 7-(2-(diethylamino)ethyl)-  
1,3-Dimethyl-7-(2-(diethylamino)ethyl)xanthine  
7-(2-(Diethylamino)ethyl)-1,3-dimethylxanthine  
7-(2-(Diethylamino)ethyl)theophylline  
Millophylline  
Dietamiphylline  
7-[2-(Diethylamino)ethyl]-3,7-dihydro-1,3-dimethyl-1H-purine-2,6-dione  
7-(Diethylaminoethyl)theophylline  
NSC 38348

**Inchi:**

InChI=1S/C13H21N5O2/c1-5-17(6-2)7-8-18-9-14-11-10(18)12(19)16(4)13(20)15(11)3/h9

**InchiKey:**

AWKLBIOQCIOBSB-UHFFFAOYSA-N

**Formula:**

C13H21N5O2

**SMILES:**

CCN(CC)CCn1cnc2c1c(=O)n(C)c(=O)n2C

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

279.34

**CAS:**

314-35-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Crippen Method
logp	-0.225		Crippen Method
mcvol	216.750	ml/mol	McGowan Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C314352&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C314352&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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