

# Pentoxifylline

**Other names:**

1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-1-(5-oxohexyl)-  
Theobromine, 1-(5-oxohexyl)-  
BL 191  
3,7-Dihydro-3,7-dimethyl-1-(5-oxohexyl)-1H-purine-2,6-dione  
Dimethyloxohexylxanthine  
3,7-Dimethyl-1-(5-oxohexyl)-1H,3H-purin-2,6-dione  
3,7-Dimethyl-1-(5-oxohexyl)xanthine  
1-(5-Oxohexyl)-3,7-dimethylxanthine  
1-(5-Oxohexyl)theobromine  
Oxpentifylline  
Pentoxifyllin  
Pentoxiphyllium  
Pentoxyphylline  
Trental  
Vazofirin  
Azupentat  
Durapental  
Rentylin  
Torental  
EHT 0202  
NSC 637086  
Pentoxiphylline  
Pentoxyfilline  
Pentoxyphyllin  
1-(5-Oxohexyl)-3,7-dimethylxanthine (pentoxifylline)

**Inchi:**

InChI=1S/C13H18N4O3/c1-9(18)6-4-5-7-17-12(19)10-11(14-8-15(10)2)16(3)13(17)20/h8

**InchiKey:**

BYPFEZZEUUWMEJ-UHFFFAOYSA-N

**Formula:**

C13H18N4O3

**SMILES:**

CC(=O)CCCCn1c(=O)c2c(ncn2C)n(C)c1=O

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

278.31

**CAS:**

6493-05-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.68		Crippen Method
logp	0.193		Crippen Method

mcvol	208.340	ml/mol	McGowan Method
rinpol	2389.00		NIST Webbook
rinpol	2420.00		NIST Webbook
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	36.60	kJ/mol	376.80	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6493056&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6493056&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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