

# tetroxoprim

**Inchi:** InChI=1S/C16H22N4O4/c1-21-4-5-24-14-12(22-2)7-10(8-13(14)23-3)6-11-9-19-16(18)20  
**InchiKey:** WSWJIZXMAUYHOE-UHFFFAOYSA-N  
**Formula:** C16H22N4O4  
**SMILES:** COCCOc1c(OC)cc(Cc2cnc(N)nc2N)cc1OC  
**Mol. weight [g/mol]:** 334.37  
**CAS:** 53808-87-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Aqueous Solubility Prediction Method
logp	1.274		Crippen Method
mvol	252.180	ml/mol	McGowan Method
tf	427.40	K	Aqueous Solubility Prediction Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	46.36	kJ/mol	423.30	NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C53808870&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

# 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>tf:</b>	Normal melting (fusion) point

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