

Trimethoprim

Other names:

2,4-Diamino-5-(3',4',5'-trimethoxybenzyl)pyrimidine
2,4-Diamino-5-(3,4,5-Trimethoxybenzyl)pyrimidine
2,4-Pyrimidinediamine, 5-[(3,4,5-trimethoxyphenyl)methyl]-
5-(3,4,5-Trimethoxybenzyl)-2,4-diaminopyrimidine
5-[(3,4,5-Trimethoxyphenyl)methyl]-2,4-pyrimidinediamine
5-[(3,4,5-Trimethoxyphenyl)methyl]-2,4-pyrimidinediamine (trimethoprim)
BW 56-72
Bactramin
Instalac
Monoprim
Monotrim
Monotrimin
NIH 204
NSC-106568
Proloprim
Pyrimidine, 2,4-diamino-5-(3,4,5-trimethoxybenzyl)-
Syraprim
Tiempe
Trimanyl
Trimethioprim
Trimethopriom
Trimetoprim
Trimogal
Trimopan
Trimpex
Triprim
Uretrim
Veltrim
Wellcoprim

Inchi:

InChI=1S/C14H18N4O3/c1-19-10-5-8(6-11(20-2)12(10)21-3)4-9-7-17-14(16)18-13(9)15/

InchiKey:

IEDVJHCEMCRBQM-UHFFFAOYSA-N

Formula:

C14H18N4O3

SMILES:

COc1cc(Cc2cnc(N)nc2N)cc(OC)c1OC

Mol. weight [g/mol]:

290.32

CAS:

738-70-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Aqueous Solubility Prediction Method
logp	1.258		Crippen Method
mcvol	218.130	ml/mol	McGowan Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		NIST Webbook
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	49.80	kJ/mol	472.90	NIST Webbook
hfust	53.65	kJ/mol	474.00	NIST Webbook

Sources

Crippen Method:

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

Solubility of Trimethoprim in Selected Pure Solvents and (Water + Solubility of Trimethoprim (TMP) in Different Organic Solvents from (278 to 330)K

<https://www.doi.org/10.1021/acs.jced.5b00616>

<https://www.doi.org/10.1021/je700497h>

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C738705&Units=SI>

Legend

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

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