

CIMETIDINE

Other names:	1-Cyano-2-methyl-3-(2-(((5-methyl-4-imidazolyl)methyl)thio)ethyl)guanidine 2-Cyano-1-methyl-3-(2-(((5-methylimidazol-4-yl)methyl)thio)ethyl)guanidine Acibilin Acinil Cimal Cimetag Cimetum Dyspamet Edalene Eureceptor FPF 1002 Gastromet Guanidine, N''-cyano-N-methyl-N'-[2-[[[(5-methyl-1H-imidazol-4-yl)methyl]thio]ethyl]- Guanidine, N-cyano-N'-methyl-N''-[2-[[[(5-methyl-1H-imidazol-4-yl)methyl]thio]ethyl]- N-Cyano-N'-methyl-N''-[2-(((5-methyl-1H-imidazol-4-yl)methyl)thio)ethyl)guanidine Peptol SKF 92334 Tagamet Tametin Tratul Ulcedin Ulcedine Ulcerfen Ulcimet Ulcofalk Ulcomedina Ulcomet Ulhys
Inchi:	InChI=1S/C10H16N6S/c1-8-9(16-7-15-8)5-17-4-3-13-10(12-2)14-6-11/h7H,3-5H2,1-2H3,
InchiKey:	AQIXAKUUQRKLND-UHFFFAOYSA-N
Formula:	C10H16N6S
SMILES:	CN/C(=N\CCSCc1nc[nH]c1C)NC#N
Mol. weight [g/mol]:	252.35

Physical Properties

Property code	Value	Unit	Source
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ie	7.70	eV	NIST Webbook
ie	8.41	eV	NIST Webbook
log10ws	-1.57		Aqueous Solubility Prediction Method
log10ws	-1.61		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.115		Crippen Method
mcvol	195.630	ml/mol	McGowan Method
tf	414.65	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C51481619&Units=SI>

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Aqueous and cosolvent solubility data for drug-like organic compounds: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/>

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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