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:	CNC(=NCCSCc1nc[nH]c1C)NC#N
Mol. weight [g/mol]:	252.34
CAS:	51481-61-9

Physical Properties

Property code	Value	Unit	Source

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	0.116		Crippen Method
mcvol	195.630	ml/mol	McGowan Method
tf	414.65	K	Aqueous Solubility Prediction Method

Sources

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

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

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

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

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

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