Betahistine

Other names:	2-Pyridineethanamine, N-methyl- Pyridine, 2-[2-(methylamino)ethyl]- [2-(2-Pyridyl)ethyl]methylamine N-Methyl-2-pyridineethylamine 2-[2-(Methylamino)ethyl]pyridine 2-(«beta»-Methylaminoethyl)pyridine PT 9 base Serc base Sinmenier (free base) Vasomotal N-Methyl-N-«beta»-(2-pyridyl)ethylamine N-Methyl-2-pyridineethanamine NSC 42617 «beta»-Histine
Inchi:	InChI=1S/C8H12N2/c1-9-7-5-8-4-2-3-6-10-8/h2-4,6,9H,5,7H2,1H3
InchiKey:	UUQMNUMQCIQDMZ-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CNCCc1ccccn1
Mol. weight [g/mol]:	136.19
CAS:	5638-76-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.65		Crippen Method
logp	0.844		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1235.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.70	K	4.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5638766&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure