2-Pyridineethanamine, N-methyl-

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]:	136.20

Physical Properties

Property code	Value	Unit	Source
af	0.4471		Cheméo Relay (1.0)
hvap	60.95	kJ/mol	Cheméo Relay (1.0)
ie	8.89	eV	Cheméo Relay (1.0)
log10ws	1.23		Cheméo Relay (1.0)
logp	0.844		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3557.63	kPa	Cheméo Relay (1.0, beta)
rinpol	1235.00		NIST Webbook
rinpol	1235.00		NIST Webbook
tb	485.73	K	Cheméo Relay (1.0)
tc	703.23	K	Cheméo Relay (1.0)
tf	268.62	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5638766&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point