MYOSMINE

Other names: Pyridine, 3-(1-pyrrolin-2-yl)-
Myosmine
2-(3-Pyridyl)-1-pyrroline
Miosmine
Inchi: InChI=1S/C9H10N2/c1-3-8(7-10-5-1)9-4-2-6-11-9/h1,3,5,7H,2,4,6H2
InchiKey: DPNGWXJMIILTBS-UHFFFAOYSA-N
Formula: C9H10N2
SMILES: c1cncc(C2=NCCC2)c1
Mol. weight [g/mol]: 146.19

Physical Properties

Property code	Value	Unit	Source
hvap	64.78	kJ/mol	Cheméo Relay (1.0)
logp	1.664		Crippen Method
mcvol	118.710	ml/mol	McGowan Method
rinpol	1427.30		NIST Webbook
tb	544.73	K	Cheméo Relay (1.0)
tf	288.88	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C532127&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvap: Enthalpy of vaporization at standard conditions

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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