

Anabasine

Other names:	Pyridine, 3-(2-piperidinyl)-, (S)- Piperidine, 2-(3-pyridyl)- (-)-Anabasine (-)-2-(3'-Pyridyl)piperidine Anabasin Anabazin Neonicotine Neonikotin (S)-(-)-Anabasine L-3-(2'-Piperidyl)pyridine Pyridine, 3-(2-piperidyl)- 3-(2-Piperidinyl)pyridine (S)-Anabasine NSC 87504
Inchi:	InChI=1S/C10H14N2/c1-2-7-12-10(5-1)9-4-3-6-11-8-9/h3-4,6,8,10,12H,1-2,5,7H2/t10-/m
InchiKey:	MTXSIJUGVMTTMU-SNVBAGLBSA-N
Formula:	C10H14N2
SMILES:	<chem>c1cncc(C2CCCCN2)c1</chem>
Mol. weight [g/mol]:	162.23
CAS:	494-52-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	1.896		Crippen Method
mccvol	137.100	ml/mol	McGowan Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	549.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	49.50	kJ/mol	448.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	0.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C494520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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