

# C10H14N2

<b>Other names:</b>	(.+-.)-anabasine 3-(2-piperidinyl)pyridine DL-anabasine
<b>Inchi:</b>	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
<b>InchiKey:</b>	MTXSIJUGVMTTMU-UHFFFAOYSA-N
<b>Formula:</b>	C10H14N2
<b>SMILES:</b>	<chem>c1cncc(C2CCCCN2)c1</chem>
<b>Mol. weight [g/mol]:</b>	162.23
<b>CAS:</b>	13078-04-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	1.896		Crippen Method
mcpvol	137.100	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	14.95	kPa	478.00	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	19.90	kPa	488.00	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	29.84	kPa	502.90	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry

pvap	49.73	kPa	523.00	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	79.59	kPa	543.50	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	99.57	kPa	555.10	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	248.35	kPa	602.50	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	398.33	kPa	631.30	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	468.91	kPa	640.70	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	498.63	kPa	644.30	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry

## Sources

Vapor pressure data of nicotine, anabasine and cotinine using Differential Scanning Calorimetry:

NIST Webbook:

Crippen Method:

<https://www.doi.org/10.1016/j.tca.2014.08.033>

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13078041&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pvap:</b>	Vapor pressure

Latest version available from:

<https://www.chemeo.com/cid/54-908-4/C10H14N2.pdf>

Generated by Cheméo on 2024-05-03 00:55:12.792745825 +0000 UTC m=+16986961.713323137.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.