

Nicotine

Other names:	«alpha»-Nicotine «alpha»-Pyridyl-«alpha»-methylpyrrolidine 2-Nicotine o-Nicotine Nicotine
Inchi:	InChI=1S/C10H14N2/c1-12-8-4-6-10(12)9-5-2-3-7-11-9/h2-3,5,7,10H,4,6,8H2,1H3
InchiKey:	AQCRXZYYMOXFAN-UHFFFAOYSA-N
Formula:	C10H14N2
SMILES:	CN1CCCC1c1ccccn1
Mol. weight [g/mol]:	162.24

Physical Properties

Property code	Value	Unit	Source
hvap	61.36	kJ/mol	Cheméo Relay (1.0)
log10ws	0.58		Cheméo Relay (1.0)
logp	1.848		Crippen Method
mcvol	137.100	ml/mol	McGowan Method
rinpol	1362.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1339.00		NIST Webbook
rinpol	1360.00		NIST Webbook

rinpol	1381.00	NIST Webbook
rinpol	1384.00	NIST Webbook
rinpol	1354.00	NIST Webbook
rinpol	1301.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1311.00	NIST Webbook
rinpol	1346.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1329.00	NIST Webbook
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ripol	1848.00	NIST Webbook
ripol	1848.00	NIST Webbook
ripol	1842.00	NIST Webbook
ripol	1865.00	NIST Webbook
ripol	1876.00	NIST Webbook
ripol	1887.00	NIST Webbook
ripol	1829.00	NIST Webbook
ripol	1829.00	NIST Webbook

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23950041&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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