

1H-Indole, 1-methyl-

Other names:	1-Methyl-1H-indole 1-Methylindole 1-Methylindole (N-) Indole, 1-methyl- N-Methylindole indole, N-methyl-
Inchi:	InChI=1S/C9H9N/c1-10-7-6-8-4-2-3-5-9(8)10/h2-7H,1H3
InchiKey:	BLRHMMGNCXNXJL-UHFFFAOYSA-N
Formula:	C9H9N
SMILES:	Cn1ccc2ccccc21
Mol. weight [g/mol]:	131.17
CAS:	603-76-9

Physical Properties

Property code	Value	Unit	Source
hvap	62.20 ± 1.60	kJ/mol	NIST Webbook
ie	7.71	eV	NIST Webbook
ie	7.74 ± 0.03	eV	NIST Webbook
ie	7.48 ± 0.01	eV	NIST Webbook
ie	7.40 ± 0.00	eV	NIST Webbook
log10ws	-4.56		Crippen Method
logp	2.178		Crippen Method
mcpol	108.730	ml/mol	McGowan Method
rinpol	1298.20		NIST Webbook
rinpol	216.62		NIST Webbook
rinpol	216.90		NIST Webbook
rinpol	1298.20		NIST Webbook
rinpol	216.62		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1270.00		NIST Webbook
ripol	2016.00		NIST Webbook
ripol	1996.00		NIST Webbook

tf	276.50	K	Vapour pressures of 1-methyl derivatives of benzimidazole, pyrazole and indole. The energy of the intermolecular hydrogen bond N-H...N
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Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.20	K	3.50	NIST Webbook
tbrp	345.70	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.29907e+01
Coeff. B	-3.78996e+03
Coeff. C	-8.29720e+01
Temperature range (K), min.	381.32
Temperature range (K), max.	576.50

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C603769&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Combined experimental and computational study of the energetics of intermolecular hydrogen bonds of 1-methyl derivatives of benzimidazole, pyrazole and indole. The energy of the intermolecular hydrogen bond N-H...N:	https://www.doi.org/10.1016/j.jct.2009.05.018
	https://www.doi.org/10.1016/j.jct.2014.04.026
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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