1H-Indole, 2-methyl-

Other names: 2-Methyl-1H-indole
2-Methylindole
Indole, 2-methyl-
Inchi: InChI=1S/C9H9N/c1-7-6-8-4-2-3-5-9(8)10-7/h2-6,10H,1H3
InchiKey: BHNHHSOHWZKFOX-UHFFFAOYSA-N
Formula: C9H9N
SMILES: Cc1cc2ccccc2[nH]1
Mol. weight [g/mol]: 131.17
CAS: 95-20-5

Physical Properties

Property code	Value	Unit	Source
hsub	88.70 ± 2.40	kJ/mol	NIST Webbook
ie	7.44 ± 0.01	eV	NIST Webbook
ie	7.67 ± 0.00	eV	NIST Webbook
ie	7.67 ± 0.00	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	1.994		Crippen Method
mcvol	108.730	ml/mol	McGowan Method
rinpol	1373.00		NIST Webbook
rinpol	237.42		NIST Webbook
rinpol	240.10		NIST Webbook
rinpol	234.59		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1385.00		NIST Webbook
ripol	2425.00		NIST Webbook
tb	543.00 ± 4.00	K	NIST Webbook
tb	545.20	K	NIST Webbook
tt	331.97	K	Thermodynamic properties of 2-methylindole: Experimental and computational results for gas-phase entropy and enthalpy of formation

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	15.72	kJ/mol	329.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47095e+01
Coeff. B	-4.56624e+03
Coeff. C	-9.27020e+01
Temperature range (K), min.	409.32
Temperature range (K), max.	578.57

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95205&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Combined experimental and computational study of the energetics of methylindoles	https://www.doi.org/10.1016/j.jct.2009.05.018
Thermodynamic properties of 2-methylindole: Experimental and computational results for gas-phase entropy and enthalpy of formation:	https://www.doi.org/10.1016/j.jct.2018.05.029
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tt:	Triple Point Temperature