

1H-Indole, 2,3-dihydro-4-methyl-

Other names:	4-Methylindoline
Inchi:	InChI=1S/C9H11N/c1-7-3-2-4-9-8(7)5-6-10-9/h2-4,10H,5-6H2,1H3
InchiKey:	BSRIUSPUGCAPHE-UHFFFAOYSA-N
Formula:	C9H11N
SMILES:	Cc1cccc2c1CCN2
Mol. weight [g/mol]:	133.19
CAS:	62108-16-1

Physical Properties

Property code	Value	Unit	Source
gf	274.22	kJ/mol	Joback Method
hf	115.45	kJ/mol	Joback Method
hfus	18.98	kJ/mol	Joback Method
hvap	46.21	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.963		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
rinpol	1479.00		NIST Webbook
rinpol	1479.00		NIST Webbook
tb	501.92	K	Joback Method
tc	736.54	K	Joback Method
tf	369.86	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.61	J/molxK	501.92	Joback Method
cpg	253.60	J/molxK	541.02	Joback Method
cpg	266.65	J/molxK	580.13	Joback Method
cpg	278.82	J/molxK	619.23	Joback Method
cpg	290.16	J/molxK	658.33	Joback Method
cpg	300.74	J/molxK	697.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62108161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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