

1H-Indole, 4-methyl-

Other names:	4-Methyl-1H-indole 4-Methylindole Indole, 4-methyl-
Inchi:	InChI=1S/C9H9N/c1-7-3-2-4-9-8(7)5-6-10-9/h2-6,10H,1H3
InchiKey:	PZOUSPYUWWUPPK-UHFFFAOYSA-N
Formula:	C9H9N
SMILES:	Cc1cccc2[nH]ccc12
Mol. weight [g/mol]:	131.17
CAS:	16096-32-5

Physical Properties

Property code	Value	Unit	Source
ie	7.60 ± 0.01	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	1.994		Crippen Method
mvol	108.730	ml/mol	McGowan Method
rinpol	237.64		NIST Webbook
tb	540.20	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47005e+01
Coeff. B	-4.52578e+03
Coeff. C	-9.13120e+01
Temperature range (K), min.	405.32
Temperature range (K), max.	573.34

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16096325&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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
tb:	Normal Boiling Point Temperature

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