1H-Indole, 6-methyl-

Other names:	6-Methylindole
	Indole, 6-methyl-
Inchi:	InChI=1S/C9H9N/c1-7-2-3-8-4-5-10-9(8)6-7/h2-6,10H,1H3
InchiKey:	ONYNOPPOVKYGRS-UHFFFAOYSA-N
Formula:	C9H9N
SMILES:	Cc1ccc2cc[nH]c2c1
Mol. weight [g/mol]:	131.17
CAS:	3420-02-8

Physical Properties

Property code	Value	Unit	Source
ie	7.54 ± 0.01	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	1.994		Crippen Method
mcvol	108.730	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.20	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39985e+01
Coeff. B	-4.20390e+03
Coeff. C	-8.74780e+01
Temperature range (K), min.	394.09
Temperature range (K), max.	571.40

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3420028&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tbrp:	Boiling point at reduced pressure