

Indole, 3-methyl-

Other names:	1H-Indole, 3-methyl- 3-MI 3-Methyl-1H-indole 3-Methylindole 3-Methylindole (skatol) 3-methylindole (skatole) Indole, 3-methyl- (skatole) NSC 122024 Scatole Skatol Skatole «beta»-Methylindole Â«betaÂ»-Methylindole
Inchi:	InChI=1S/C9H9N/c1-7-6-10-9-5-3-2-4-8(7)9/h2-6,10H,1H3
InchiKey:	ZFRKQXVRDFCRJG-UHFFFAOYSA-N
Formula:	C9H9N
SMILES:	Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	131.17
CAS:	83-34-1

Physical Properties

Property code	Value	Unit	Source
hsub	90.40 ± 1.90	kJ/mol	NIST Webbook
ie	7.51 ± 0.00	eV	NIST Webbook
ie	7.51 ± 0.00	eV	NIST Webbook
ie	7.54 ± 0.01	eV	NIST Webbook
log10ws	-2.42		Aqueous Solubility Prediction Method
log10ws	-2.42		Estimated Solubility Method
logp	1.994		Crippen Method
mcvol	108.730	ml/mol	McGowan Method
rinpol	1389.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1399.00		NIST Webbook

rinpol	1391.00	NIST Webbook
rinpol	1395.00	NIST Webbook
rinpol	1401.00	NIST Webbook
rinpol	1390.00	NIST Webbook
rinpol	1391.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1394.00	NIST Webbook
rinpol	1398.00	NIST Webbook
rinpol	1396.00	NIST Webbook
rinpol	1400.00	NIST Webbook
rinpol	1381.00	NIST Webbook
rinpol	1382.00	NIST Webbook
rinpol	1396.00	NIST Webbook
rinpol	1399.00	NIST Webbook
rinpol	1351.00	NIST Webbook
rinpol	1354.00	NIST Webbook
rinpol	1408.00	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1427.00	NIST Webbook
rinpol	1374.00	NIST Webbook
rinpol	1401.00	NIST Webbook
rinpol	1362.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1339.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1351.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1387.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1402.00	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1390.00	NIST Webbook
rinpol	1365.00	NIST Webbook
rinpol	1365.00	NIST Webbook
rinpol	237.80	NIST Webbook
rinpol	239.20	NIST Webbook
rinpol	236.66	NIST Webbook
rinpol	1381.00	NIST Webbook
rinpol	237.88	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1380.00	NIST Webbook

ripol	1410.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	237.80		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	2486.00		NIST Webbook
ripol	2489.00		NIST Webbook
ripol	2496.00		NIST Webbook
ripol	2468.00		NIST Webbook
ripol	2477.00		NIST Webbook
ripol	2505.00		NIST Webbook
ripol	2492.00		NIST Webbook
ripol	2503.00		NIST Webbook
ripol	2504.00		NIST Webbook
ripol	2514.00		NIST Webbook
ripol	2523.00		NIST Webbook
ripol	2489.00		NIST Webbook
ripol	2484.00		NIST Webbook
ripol	2500.00		NIST Webbook
ripol	2459.00		NIST Webbook
ripol	2490.00		NIST Webbook
ripol	2500.00		NIST Webbook
ripol	2530.00		NIST Webbook
ripol	2495.00		NIST Webbook
ripol	2510.00		NIST Webbook
ripol	2484.00		NIST Webbook
ripol	2495.00		NIST Webbook
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ripol	2468.00		NIST Webbook
ripol	2452.00		NIST Webbook
ripol	2516.00		NIST Webbook
ripol	2489.00		NIST Webbook
ripol	2489.00		NIST Webbook
ripol	2504.00		NIST Webbook
ripol	2520.00		NIST Webbook
ripol	2494.00		NIST Webbook
tf	368.25 ± 0.60	K	NIST Webbook
tf	369.32	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	83.30	kJ/mol	310.50	NIST Webbook
hvapt	64.50	kJ/mol	454.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	538.70	K	101.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47363e+01
Coeff. B	-4.52946e+03
Coeff. C	-9.10340e+01
Temperature range (K), min.	370.65
Temperature range (K), max.	571.62

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C83341&Units=SI>

The Yaws Handbook of Vapor <https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Pressure:
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Combined experimental and computational study of the energetics of methylindoles: <https://www.doi.org/10.1016/j.jct.2009.05.018>

Legend

hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
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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