

1H-Indole, 1-ethyl-

Other names:	1-Ethyl-1H-indole 1-Ethylindole Indole, 1-ethyl- N-Ethylindole
Inchi:	InChI=1S/C10H11N/c1-2-11-8-7-9-5-3-4-6-10(9)11/h3-8H,2H2,1H3
InchiKey:	QRRKZFCXXBFHSV-UHFFFAOYSA-N
Formula:	C10H11N
SMILES:	CCn1ccc2ccccc21
Mol. weight [g/mol]:	145.20
CAS:	10604-59-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	2.661		Crippen Method
mcvol	122.820	ml/mol	McGowan Method
ripol	1340.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2036.00		NIST Webbook
ripol	2020.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.27222e+01
Coeff. B	-3.81046e+03
Coeff. C	-8.72810e+01
Temperature range (K), min.	378.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10604598&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.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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