3-ethyl-indole

Other names: 3-ethyl-1H-indole
Inchi: InChI=1S/C10H11N/c1-2-8-7-11-10-6-4-3-5-9(8)10/h3-7,11H,2H2,1H3
InchiKey: GOVXKUCVZUROAN-UHFFFAOYSA-N
Formula: C10H11N
SMILES: CCc1c[nH]c2ccccc12
Mol. weight [g/mol]: 145.20
CAS: 1484-19-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	2.248		Crippen Method
mcvol	122.820	ml/mol	McGowan Method
rinpol	1493.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1479.00		NIST Webbook
ripol	2509.00		NIST Webbook
ripol	2540.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43476e+01
Coeff. B	-4.50302e+03
Coeff. C	-9.46480e+01
Temperature range (K), min.	414.92
Temperature range (K), max.	592.99

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1484191&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/ci990307l
Crippen Method:	https://www.chemeo.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