1H-Pyrrole, 2-ethyl-

Other names:	2-Ethylpyrrole
	2-ethyl-1H-pyrrole
	Pyrrole,2-ethyl-
Inchi:	InChI=1S/C6H9N/c1-2-6-4-3-5-7-6/h3-5,7H,2H2,1H3
InchiKey:	XRPDDDRNQJNHLQ-UHFFFAOYSA-N
Formula:	C6H9N
SMILES:	CCc1ccc[nH]1
Mol. weight [g/mol]:	95.14
CAS:	1551-06-0

Physical Properties

Property code	Value	Unit	Source
ie	7.97 ± 0.05	eV	NIST Webbook
log10ws	-1.49		Crippen Method
logp	1.095		Crippen Method
mcvol	85.920	ml/mol	McGowan Method
rinpol	934.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	941.00		NIST Webbook
tb	437.20	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	437.70	K	101.00	NIST Webbook
tbrp	332.70	K	2.00	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50353e+01
Coeff. B	-3.90140e+03
Coeff. C	-6.26780e+01
Temperature range (K), min.	327.22
Temperature range (K), max.	463.90

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1551060&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

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
tbrp:	Boiling point at reduced pressure