

1H-Pyrrole, 1-ethyl-

Other names:	1-Ethylpyrrole 1-ethyl-1H-pyrrole N-Ethylpyrrole Pyrrole, 1-ethyl-
Inchi:	InChI=1S/C6H9N/c1-2-7-5-3-4-6-7/h3-6H,2H2,1H3
InchiKey:	VPUAYOJTHRDUTK-UHFFFAOYSA-N
Formula:	C6H9N
SMILES:	CCn1cccc1
Mol. weight [g/mol]:	95.14
CAS:	617-92-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.73		Crippen Method
logp	1.508		Crippen Method
mcvol	85.920	ml/mol	McGowan Method
rinpol	803.00		NIST Webbook
rinpol	803.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	829.00		NIST Webbook
ripol	1178.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1178.00		NIST Webbook

ripol	1184.00		NIST Webbook
ripol	1184.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1168.00		NIST Webbook
ripol	1157.00		NIST Webbook
ripol	1181.00		NIST Webbook
tb	403.55 ± 0.50	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48913e+01
Coeff. B	-3.60030e+03
Coeff. C	-5.30870e+01
Temperature range (K), min.	279.65
Temperature range (K), max.	428.91

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=C617925&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tb: Normal Boiling Point Temperature

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