2-Ethylpiperidine

Other names:	Piperidine, 2-ethyl-
	coniine
	«alpha»-Ethylpiperidine
	Â«alphaÂ»-Ethylpiperidine
Inchi:	InChI=1S/C7H15N/c1-2-7-5-3-4-6-8-7/h7-8H,2-6H2,1H3
InchiKey:	QBBKKFZGCDJDQK-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	CCC1CCCCN1
Mol. weight [g/mol]:	113.20
CAS:	1484-80-6

Physical Properties

Property code	Value	Unit	Source
gf	120.22	kJ/mol	Joback Method
hf	-95.68	kJ/mol	Joback Method
hfus	15.31	kJ/mol	Joback Method
hvap	42.20 ± 0.90	kJ/mol	NIST Webbook
log10ws	-1.50		Aqueous Solubility Prediction Method
logp	1.538		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	890.00		NIST Webbook
rinpol	890.00		NIST Webbook
tb	416.20	K	NIST Webbook
tc	639.14	K	Joback Method
tf	281.06	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.15	J/mol×K	427.66	Joback Method
cpg	231.73	J/mol×K	462.91	Joback Method

cpg	247.54	J/mol×K	498.15	Joback Method
cpg	262.60	J/mol×K	533.40	Joback Method
cpg	276.91	J/mol×K	568.65	Joback Method
cpg	290.49	J/mol×K	603.89	Joback Method
cpg	303.36	J/mol×K	639.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40920e+01
Coeff. B	-3.40828e+03
Coeff. C	-5.64370e+01
Temperature range (K), min.	303.33
Temperature range (K), max.	444.60

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1484806&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

Legend

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume