Piperidine, 5-ethyl-2-methyl-

Other names:	2-Methyl-5-ethylpiperidine
	2-Pipecoline, 5-ethyl-
	3-Ethyl-6-methylpiperidine
	5-Ethyl-2-methylpiperidine
	5-Ethyl-2-pipecoline
	Copellidin
	Copellidine
Inchi:	InChI=1S/C8H17N/c1-3-8-5-4-7(2)9-6-8/h7-9H,3-6H2,1-2H3
InchiKey:	XOFNHZHCGBPVGJ-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	CCC1CCC(C)NC1
Mol. weight [g/mol]:	127.23
CAS:	104-89-2

Physical Properties

Property code	Value	Unit	Source
gf	120.93	kJ/mol	Joback Method
hf	-136.66	kJ/mol	Joback Method
hfus	18.97	kJ/mol	Joback Method
hvap	40.28	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.785		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
tb	445.87	K	Joback Method
tc	654.36	K	Joback Method
tf	258.30 ± 0.60	K	NIST Webbook
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.15	J/mol×K	445.87	Joback Method
cpg	276.16	J/mol×K	480.62	Joback Method

cpg	293.37	J/mol×K	515.37	Joback Method
cpg	309.79	J/mol×K	550.12	Joback Method
cpg	325.44	J/mol×K	584.86	Joback Method
cpg	340.31	J/mol×K	619.61	Joback Method
cpg	354.42	J/mol×K	654.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54268e+01
Coeff. B	-3.95062e+03
Coeff. C	-6.36950e+01
Temperature range (K), min.	324.65
Temperature range (K), max.	454.25

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104892&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume