Piperidine, 4-methyl-

Other names:	4-Methylpiperidine
	4-Pipecoline
	«gamma»-Pipecoline
	Â«gammaÂ»-Pipecoline
Inchi:	InChI=1S/C6H13N/c1-6-2-4-7-5-3-6/h6-7H,2-5H2,1H3
InchiKey:	UZOFELREXGAFOI-UHFFFAOYSA-N
Formula:	C6H13N
SMILES:	CC1CCNCC1
Mol. weight [g/mol]:	99.17
CAS:	626-58-4

Physical Properties

Property code	Value	Unit	Source
gf	111.80	kJ/mol	Joback Method
hf	-75.04	kJ/mol	Joback Method
hfus	12.72	kJ/mol	Joback Method
hvap	40.60 ± 0.90	kJ/mol	NIST Webbook
ie	8.01 ± 0.05	eV	NIST Webbook
ie	8.06 ± 0.05	eV	NIST Webbook
log10ws	-1.18		Crippen Method
logp	1.006		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
pc	4088.15	kPa	Joback Method
rinpol	831.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	816.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1077.00		NIST Webbook
ripol	1077.00		NIST Webbook
tb	399.15 ± 1.50	K	NIST Webbook
tb	397.20	K	NIST Webbook
tb	406.20	K	NIST Webbook
tc	618.71	K	Joback Method
tf	269.79	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.55	J/mol×K	404.78	Joback Method
cpg	189.85	J/mol×K	440.43	Joback Method
cpg	204.46	J/mol×K	476.09	Joback Method
cpg	218.38	J/mol×K	511.74	Joback Method
cpg	231.63	J/mol×K	547.40	Joback Method
cpg	244.20	J/mol×K	583.05	Joback Method
cpg	256.13	J/mol×K	618.71	Joback Method
cpl	209.00	J/mol×K	298.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48664e+01
Coeff. B	-3.52507e+03
Coeff. C	-5.32260e+01
Temperature range (K), min.	295.02
Temperature range (K), max.	422.15

Sources

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=C626584&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
Thermodynamic Study of Four {Methylpiperidine + Water} Systems: New Experimental Data and Challenging Modeling for the Simultaneous Representation of Liquid-Liquid Equilibrium and Energetic Properties:	https://www.doi.org/10.1021/acs.jced.8b00974

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume