2-Methylpiperidine

Other names:	.alpha.-methylpiperidine
	2-PIPECOLINE
	ALPHA-METHYLPIPERIDINE
	Pipecoline, «alpha»
	Pipecoline, Â«alphaÂ»
	Piperidine, 2-methyl-
	Pipicoline
	«alpha»-Methylpiperidine
	«alpha»-Pipecolin
	«alpha»-Pipecoline
	Â«alphaÂ»-Methylpiperidine
	Â«alphaÂ»-Pipecolin
	Â«alphaÂ»-Pipecoline
Inchi:	InChI=1S/C6H13N/c1-6-4-2-3-5-7-6/h6-7H,2-5H2,1H3
InchiKey:	NNWUEBIEOFQMSS-UHFFFAOYSA-N
Formula:	C6H13N
SMILES:	CC1CCCCN1
Mol. weight [g/mol]:	99.17
CAS:	109-05-7

Physical Properties

Property code	Value	Unit	Source
af	0.2690		KDB
chl	-4094.00 ± 1.00	kJ/mol	NIST Webbook
gf	111.80	kJ/mol	Joback Method
hf	-84.50 ± 1.10	kJ/mol	NIST Webbook
hfl	-124.90 ± 1.10	kJ/mol	NIST Webbook
hfus	12.72	kJ/mol	Joback Method
hvap	40.40	kJ/mol	NIST Webbook
hvap	40.50 ± 0.20	kJ/mol	NIST Webbook
ie	7.90 ± 0.10	eV	NIST Webbook
ie	7.76 ± 0.05	eV	NIST Webbook
ie	8.04 ± 0.05	eV	NIST Webbook
log10ws	-1.53		Crippen Method
logp	1.148		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
pc	3800.00	kPa	KDB

rinpol	793.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	810.00		NIST Webbook
ripol	1017.00		NIST Webbook
ripol	1017.00		NIST Webbook
ripol	1027.00		NIST Webbook
sl	243.76	J/mol×K	NIST Webbook
sl	243.75	J/mol×K	NIST Webbook
sl	243.75	J/mol×K	NIST Webbook
tb	391.40	K	KDB
tb	391.15 ± 1.50	K	NIST Webbook
tc	598.00	K	KDB
tf	269.36	K	NIST Webbook
tt	269.35 ± 0.00	K	NIST Webbook
tt	269.31 ± 0.03	K	NIST Webbook
tt	269.35 ± 0.10	K	NIST Webbook
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	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	256.13	J/mol×K	618.71	Joback Method
cpg	244.20	J/mol×K	583.05	Joback Method
cpg	189.85	J/mol×K	440.43	Joback Method
cpl	221.03	J/mol×K	318.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions

cpl	221.40	J/mol×K	323.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	222.07	J/mol×K	328.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	220.18	J/mol×K	313.16	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	212.97	J/mol×K	298.15	NIST Webbook
cpl	212.96	J/mol×K	298.15	NIST Webbook
cpl	212.97	J/mol×K	298.15	NIST Webbook
cpl	205.00	J/mol×K	298.00	NIST Webbook
cpl	219.60	J/mol×K	308.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	218.99	J/mol×K	303.16	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions

cpl	218.00	J/mol×K	298.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	217.34	J/mol×K	293.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	216.85	J/mol×K	288.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	222.76	J/mol×K	333.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	215.38	J/mol×K	283.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
hfust	18.58	kJ/mol	269.40	NIST Webbook
hfust	18.58	kJ/mol	269.40	NIST Webbook
hfust	18.58	kJ/mol	269.36	NIST Webbook
hfust	18.58	kJ/mol	269.36	NIST Webbook
hvapt	38.20	kJ/mol	377.00	NIST Webbook

rhol	846.70	kg/m3	288.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems
rhol	826.08	kg/m3	308.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems
rhol	817.35	kg/m3	318.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems
rhol	809.08	kg/m3	328.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems
rhol	801.96	kg/m3	338.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems
rhol	835.79	kg/m3	298.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	391.70	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42689e+01
Coeff. B	-3.30031e+03
Coeff. C	-5.01680e+01
Temperature range (K), min.	269.45
Temperature range (K), max.	418.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.37431e+01
Coeff. B	-5.16582e+03
Coeff. C	-2.67791e+00
Coeff. D	5.93169e-07
Temperature range (K), min.	571.15
Temperature range (K), max.	703.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Liquid-liquid phase separation of {amine e H2O e CO2} systems: New methods for key data:	https://www.doi.org/10.1016/j.fluid.2016.10.010
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109057&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1350
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems:	https://www.doi.org/10.1016/j.fluid.2010.05.001
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1350
Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions:	https://www.doi.org/10.1021/je5008444
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume