2-Pentanol, 4-methyl-

Other names:	(.+/-.)-4-Methyl-2-pentanol
	1,3-Dimethyl-1-butanol
	1,3-Dimethylbutanol
	2-Methyl-4-Pentanol
	3-MIC
	4-Methyl-2-amyl alcohol
	4-Methyl-2-pentanol
	4-Methyl-2-pentyl alcohol
	4-Methylpentan-2-ol
	4-Methylpentanol-2
	4-Metilpentan-2-olo
	4-Pentanol, 2-methyl-
	Alcool methyl amylique
	Isobutylmethylcarbinol
	Isobutylmethylmethanol
	MAOH
	MIBC
	MIC
	Methyl amyl alcohol
	Methyl-isobutylkarbinol
	Methylisobutylcarbinol
	Metilamil alcohol
	NSC 9384
	UN 2053
	dl-Methylisobutylcarbinol
Inchi:	InChI=1S/C6H14O/c1-5(2)4-6(3)7/h5-7H,4H2,1-3H3
InchiKey:	WVYWICLMDOOCFB-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CC(C)CC(C)O
Mol. weight [g/mol]:	102.17
CAS:	108-11-2

Physical Properties

Property code	Value	Unit	Source
gf	-142.06	kJ/mol	Joback Method
hf	-344.10 ± 2.10	kJ/mol	NIST Webbook

hfl	-394.70 ± 0.75	kJ/mol	NIST Webbook
hfus	8.34	kJ/mol	Joback Method
hvap	57.30 ± 0.30	kJ/mol	NIST Webbook
log10ws	-0.80		Aqueous Solubility Prediction Method
log10ws	-0.80		Estimated Solubility Method
logp	1.413		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	744.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	759.40		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	775.50		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	774.40		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	744.00		NIST Webbook
ripol	1173.00		NIST Webbook
ripol	1203.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1173.00		NIST Webbook
ripol	1168.00		NIST Webbook
ripol	1168.00		NIST Webbook
ripol	1168.00		NIST Webbook

ripol	1170.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1172.00		NIST Webbook
ripol	1171.00		NIST Webbook
ripol	1167.00		NIST Webbook
tb	404.80	K	KDB
tc	574.40	K	KDB
tc	574.40 ± 0.50	K	NIST Webbook
tc	574.40 ± 0.50	K	NIST Webbook
tf	183.00	K	KDB
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.50	J/mol×K	568.09	Joback Method
cpg	207.81	J/mol×K	427.98	Joback Method
cpg	217.90	J/mol×K	456.00	Joback Method
cpg	227.60	J/mol×K	484.02	Joback Method
cpg	236.93	J/mol×K	512.04	Joback Method
cpg	245.89	J/mol×K	540.06	Joback Method
cpg	262.76	J/mol×K	596.11	Joback Method
cpl	272.34	J/mol×K	298.15	NIST Webbook
cpl	273.01	J/mol×K	298.15	NIST Webbook
dvisc	0.0015500	Pa×s	323.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
dvisc	0.0032300	Pa×s	303.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
dvisc	0.0022400	Pa×s	313.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
hvapt	45.60	kJ/mol	350.50	NIST Webbook
hvapt	59.60	kJ/mol	267.50	NIST Webbook

hvapt	47.30	kJ/mol	378.50	NIST Webbook
hvapt	49.60	kJ/mol	349.50	NIST Webbook
rfi	1.41010		298.20	Experimental and modeling study of liquid phase equilibria for (water + phosphoric acid + sec-alcohols) systems

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53762e+01
Coeff. B	-3.73911e+03
Coeff. C	-5.74310e+01
Temperature range (K), min.	305.24
Temperature range (K), max.	428.94

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.02379e+02
Coeff. B	-9.41712e+03
Coeff. C	-1.25868e+01
Coeff. D	6.49625e-06
Temperature range (K), min.	183.00
Temperature range (K), max.	574.40

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=836
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108112&Units=SI
Measurement and Thermodynamic Models for Ternary Liquid-Liquid Equilibrium Systems {Water + Polyoxymethylene Dimethyl Ethers + 4-Methyl-2-pentanol} at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.8b00323
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid−Liquid Equilibrium in the Ternary Systems Water + Cyclohexanone + Benzene or Methyl Isobutyl Carbinol at 303.15 and 323.15 K: Experimental Data and Correlation:	https://www.doi.org/10.1021/acs.jced.7b00511
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Liquid-Liquid Equilibrium Measurements for the Ternary System of Water + Cyclohexanol + Methyl Isobutyl Ketone at Various Temperatures:	https://www.doi.org/10.1021/acs.jced.9b00290
Liquid-Liquid Equilibria for the Ternary Systems Water + Cyclohexanol + 2-Methyl-1-pentanol at Various Temperatures and Water + Cyclohexanol + Methyl Isobutyl Ketone at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00683
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems:	https://www.doi.org/10.1021/je0498053
Experimental and modeling study of liquid phase equilibria for (water + phosphoric acid + see alcohols) systems:	https://www.doi.org/10.1016/j.jct.2019.04.005
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=836
Measurement and Thermodynamic Modeling of Ternary (Liquid + Liquid) Equilibrium for Extraction of N,N-Dimethylacetamide from Aqueous Solution with Different Solvents:	https://www.doi.org/10.1021/acs.jced.7b00194
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Liquid-liquid equilibria for the extraction of furfural from aqueous solution using different solvents:	https://www.doi.org/10.1016/j.fluid.2016.06.040
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Liquid Liquid Equilibria for the Ternary Systems of Water + Butane-2,3-diol + 2-Methylbutan-1-ol, 2-Methylbutan-2-ol, and 4-Methylpentan-2-ol at 298.15 and 308.15 K:	https://www.doi.org/10.1021/acs.jced.6b00945
Liquid-liquid equilibrium study for ternary systems of water + propargyl alcohol + 1-butanol or 2-butanol at 298.15 and 308.15 K:	https://www.doi.org/10.1016/j.jct.2019.03.033
Solubility in Binary Solvent Mixtures: Measurement and Thermodynamic Modeling:	https://www.doi.org/10.1021/je020216b
Naphthalene Dissolved in Alcohol + Acetonitrile Mixtures at 298.2 K:	

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
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

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