1-Pentanol, 2-methyl-

Other names:	2-Methyl-1-pentanol
	2-Methyl-2-propylethanol
	2-Methylpentanol
	2-Methylpentanol-1
	2-methylpentan-1-ol
	2-methylpentyl alcohol
	AMYL METHYL ALCOHOL
	ISOPROPYL DIMETHYL CARBINOL
	Isohexyl alcohol
	M.I.B.C.
	Methyl-2 pentanol-1
Inchi:	InChI=1S/C6H14O/c1-3-4-6(2)5-7/h6-7H,3-5H2,1-2H3
InchiKey:	PFNHSEQQEPMLNI-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCCC(C)CO
Mol. weight [g/mol]:	102.17
CAS:	105-30-6

Physical Properties

Property code	Value	Unit	Source
gf	-139.62	kJ/mol	Joback Method
hf	-324.68	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	59.40 ± 0.30	kJ/mol	NIST Webbook
log10ws	-1.11		Aqueous Solubility Prediction Method
log10ws	-1.11		Estimated Solubility Method
logp	1.415		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3450.00 ± 50.00	kPa	NIST Webbook
pc	3450.00	kPa	KDB
pc	3450.00 ± 20.00	kPa	NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	837.00		NIST Webbook

rinpol	846.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	132.61		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	803.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	837.50		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	836.20		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1293.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1268.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1247.00		NIST Webbook
tb	428.42	K	Joback Method
tc	604.40 ± 0.50	K	NIST Webbook
tc	604.40	K	KDB
tc	604.40 ± 0.70	K	NIST Webbook
tf	203.20	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.25	J/mol×K	592.97	Joback Method
cpg	217.54	J/mol×K	455.85	Joback Method
cpg	207.74	J/mol×K	428.42	Joback Method
cpg	253.18	J/mol×K	565.55	Joback Method
cpg	244.78	J/mol×K	538.12	Joback Method
cpg	236.05	J/mol×K	510.70	Joback Method
cpg	226.97	J/mol×K	483.27	Joback Method
cpl	247.63	J/mol×K	298.15	NIST Webbook
cpl	248.40	J/mol×K	298.15	NIST Webbook
cpl	249.21	J/mol×K	298.15	NIST Webbook
dvisc	0.0022500	Pa×s	323.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
dvisc	0.0031800	Pa×s	313.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
dvisc	0.0045500	Pa×s	303.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
hvapt	55.70 ± 0.20	kJ/mol	343.00	NIST Webbook
hvapt	57.40 ± 0.20	kJ/mol	328.00	NIST Webbook
hvapt	64.90	kJ/mol	277.50	NIST Webbook
hvapt	49.30	kJ/mol	395.00	NIST Webbook
hvapt	52.70 ± 0.20	kJ/mol	368.00	NIST Webbook
hvapt	54.20	kJ/mol	360.50	NIST Webbook
hvapt	50.20	kJ/mol	355.50	NIST Webbook
hvapt	53.90 ± 0.20	kJ/mol	358.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61826e+01
Coeff. B	-4.25182e+03
Coeff. C	-5.33290e+01
Temperature range (K), min.	320.82
Temperature range (K), max.	444.44

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.09496e+01
Coeff. B	-7.82259e+03
Coeff. C	-4.56500e+00
Coeff. D	-9.57195e-07
Temperature range (K), min.	223.00
Temperature range (K), max.	582.00

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C105306&Units=SI

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

Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems: https://www.doi.org/10.1021/je0498053

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=835

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

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

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Solubility in Binary Solvent Mixtures: https://www.doi.org/10.1021/je020216b

Anthracene Dissolved in Alcohol + Acetonitrile Mixtures at 298.2 K: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=835

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
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
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