2-Pentanol, 2-methyl-

Other names:	1,1-Dimethylbutanol
	2-Hydroxy-2-methylpentane
	2-Methyl-2-hydroxypentane
	2-Methyl-2-pentanol
	2-Methylpentan-2-ol
	Methyl-2 pentanol-2
	UN 2560
	dimethylpropylcarbinol
Inchi:	InChI=1S/C6H14O/c1-4-5-6(2,3)7/h7H,4-5H2,1-3H3
InchiKey:	WFRBDWRZVBPBDO-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCCC(C)(C)O
Mol. weight [g/mol]:	102.17
CAS:	590-36-3

Physical Properties

Property code	Value	Unit	Source
gf	-134.34	kJ/mol	Joback Method
hf	-328.15	kJ/mol	Joback Method
hfus	7.97	kJ/mol	Joback Method
hvap	54.82	kJ/mol	NIST Webbook
hvap	54.70 ± 0.20	kJ/mol	NIST Webbook
log10ws	-0.49		Estimated Solubility Method
log10ws	-0.49		Aqueous Solubility Prediction Method
logp	1.557		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	718.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	718.00		NIST Webbook

rinpol	720.00	NIST Webbook
rinpol	704.00	NIST Webbook
rinpol	726.00	NIST Webbook
rinpol	719.00	NIST Webbook
rinpol	718.00	NIST Webbook
rinpol	725.00	NIST Webbook
rinpol	690.20	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	690.90	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	722.30	NIST Webbook
rinpol	723.40	NIST Webbook
rinpol	735.00	NIST Webbook
rinpol	722.00	NIST Webbook
rinpol	707.00	NIST Webbook
rinpol	717.00	NIST Webbook
rinpol	688.80	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	716.00	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	722.00	NIST Webbook
rinpol	716.00	NIST Webbook
rinpol	718.00	NIST Webbook
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rinpol	717.00	NIST Webbook
rinpol	718.00	NIST Webbook
rinpol	725.00	NIST Webbook
rinpol	718.00	NIST Webbook
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rinpol	718.00	NIST Webbook
rinpol	717.00	NIST Webbook
rinpol	718.00	NIST Webbook
rinpol	718.00	NIST Webbook
rinpol	723.00	NIST Webbook
ripol	1087.00	NIST Webbook
ripol	1101.00	NIST Webbook
ripol	1110.00	NIST Webbook
ripol	1090.00	NIST Webbook
ripol	1094.00	NIST Webbook
ripol	1079.00	NIST Webbook
ripol	1114.00	NIST Webbook
ripol	1112.00	NIST Webbook
ripol	1097.00	NIST Webbook

ripol	1101.00		NIST Webbook
ripol	1101.00		NIST Webbook
tb	395.95 ± 1.00	K	NIST Webbook
tb	395.65 ± 1.00	K	NIST Webbook
tb	393.15 ± 2.00	K	NIST Webbook
tb	394.65 ± 1.00	K	NIST Webbook
tb	394.20	K	NIST Webbook
tb	393.65 ± 2.00	K	NIST Webbook
tb	394.24 ± 0.20	K	NIST Webbook
tb	396.65 ± 4.00	K	NIST Webbook
tb	392.65 ± 4.00	K	NIST Webbook
tb	396.15 ± 2.00	K	NIST Webbook
tb	395.50 ± 1.00	K	NIST Webbook
tb	395.45 ± 2.00	K	NIST Webbook
tb	394.65 ± 2.00	K	NIST Webbook
tb	395.15 ± 1.00	K	NIST Webbook
tb	397.15 ± 1.00	K	NIST Webbook
tb	394.20	K	NIST Webbook
tb	395.15 ± 2.00	K	NIST Webbook
tb	394.65 ± 2.00	K	NIST Webbook
tb	395.00 ± 2.00	K	NIST Webbook
tc	559.50	K	NIST Webbook
tc	559.50 ± 0.70	K	NIST Webbook
tc	559.50 ± 0.70	K	NIST Webbook
tf	170.48	K	Aqueous Solubility Prediction Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.32	J/mol×K	511.13	Joback Method
cpg	230.71	J/mol×K	482.63	Joback Method
cpg	220.61	J/mol×K	454.13	Joback Method
cpg	266.42	J/mol×K	596.64	Joback Method
cpg	258.15	J/mol×K	568.14	Joback Method
cpg	249.46	J/mol×K	539.64	Joback Method
cpg	210.01	J/mol×K	425.63	Joback Method
cpl	289.03	J/mol×K	298.15	NIST Webbook

dvisc	0.0020600	Pa×s	313.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
dvisc	0.0014600	Pa×s	323.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
dvisc	0.0029300	Pa×s	303.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
hvapt	58.30	kJ/mol	342.00	NIST Webbook
hvapt	44.40 ± 0.20	kJ/mol	368.00	NIST Webbook
hvapt	51.30	kJ/mol	342.00	NIST Webbook
hvapt	39.59	kJ/mol	394.20	NIST Webbook
hvapt	44.20	kJ/mol	368.50	NIST Webbook
hvapt	48.90	kJ/mol	363.50	NIST Webbook
hvapt	46.10 ± 0.20	kJ/mol	358.00	NIST Webbook
hvapt	48.50 ± 0.20	kJ/mol	343.00	NIST Webbook
hvapt	50.70 ± 0.20	kJ/mol	328.00	NIST Webbook
hvapt	52.80 ± 0.20	kJ/mol	313.00	NIST Webbook
hvapt	49.10	kJ/mol	331.00	NIST Webbook
rhol	793.50	kg/m3	323.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
rhol	802.40	kg/m3	313.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
rhol	810.80	kg/m3	303.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems

Sources

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
Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems:	https://www.doi.org/10.1021/je0498053
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590363&Units=SI

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
rhol:	Liquid Density
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