1-Pentanol, 4-methyl-

Other names:	2-Methyl-5-pentanol
	4-Methyl-1-pentanol
	4-Methylpentan-1-ol
	4-Methylpentanol
	Isohexanol
	Isohexyl alcohol
	Pentanol, 4-methyl-
Inchi:	InChI=1S/C6H14O/c1-6(2)4-3-5-7/h6-7H,3-5H2,1-2H3
InchiKey:	PCWGTDULNUVNBN-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CC(C)CCCO
Mol. weight [g/mol]:	102.17
CAS:	626-89-1

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	60.47	kJ/mol	NIST Webbook
log10ws	-1.14		Aqueous Solubility Prediction Method
log10ws	-1.14		Estimated Solubility Method
logp	1.415		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	827.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	839.00		NIST Webbook

rinpol	846.20	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	847.00	NIST Webbook
rinpol	851.00	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	837.00	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	866.00	NIST Webbook
rinpol	845.00	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	833.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	875.00	NIST Webbook
rinpol	851.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	846.20	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	866.00	NIST Webbook
rinpol	875.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	852.60	NIST Webbook
rinpol	851.00	NIST Webbook
rinpol	827.00	NIST Webbook
ripol	1299.00	NIST Webbook
ripol	1333.00	NIST Webbook
ripol	1297.00	NIST Webbook
ripol	1284.00	NIST Webbook
ripol	1298.00	NIST Webbook
ripol	1301.00	NIST Webbook
ripol	1316.00	NIST Webbook
ripol	1318.00	NIST Webbook
ripol	1316.00	NIST Webbook
ripol	1317.00	NIST Webbook
ripol	1325.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1312.00	NIST Webbook
ripol	1318.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1301.00	NIST Webbook

ripol	1329.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1311.00		NIST Webbook
ripol	1301.00		NIST Webbook
ripol	1301.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1301.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1314.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1316.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1298.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1299.00		NIST Webbook
tb	424.80	K	NIST Webbook
tb	435.70	K	NIST Webbook
tb	421.00 ± 4.00	K	NIST Webbook
tb	420.65 ± 3.00	K	NIST Webbook
tb	425.45 ± 0.50	K	NIST Webbook
tb	421.15 ± 2.00	K	NIST Webbook
tb	421.65 ± 3.00	K	NIST Webbook
tb	420.65 ± 2.00	K	NIST Webbook
tb	420.65 ± 3.00	K	NIST Webbook
tb	425.15 ± 2.00	K	NIST Webbook
tb	424.78 ± 0.20	K	NIST Webbook
tb	424.15 ± 2.00	K	NIST Webbook
tb	424.75 ± 1.00	K	NIST Webbook
tb	425.35 ± 0.50	K	NIST Webbook

tb	425.00	K	NIST Webbook
tb	426.15 ± 2.00	K	NIST Webbook
tc	603.50 ± 0.70	K	NIST Webbook
tc	603.50	K	NIST Webbook
tc	603.50	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	207.74	J/mol×K	428.42	Joback Method
cpg	217.54	J/mol×K	455.85	Joback Method
cpg	226.97	J/mol×K	483.27	Joback Method
cpg	236.05	J/mol×K	510.70	Joback Method
cpg	244.78	J/mol×K	538.12	Joback Method
cpg	253.18	J/mol×K	565.55	Joback Method
cpg	261.25	J/mol×K	592.97	Joback Method
dvisc	0.0002400	Pa×s	428.42	Joback Method
dvisc	0.0289027	Pa×s	240.74	Joback Method
dvisc	0.2179366	Pa×s	203.20	Joback Method
dvisc	0.0021472	Pa×s	315.81	Joback Method
dvisc	0.0008856	Pa×s	353.35	Joback Method
dvisc	0.0004330	Pa×s	390.88	Joback Method
dvisc	0.0066108	Pa×s	278.27	Joback Method
hvapt	44.46	kJ/mol	425.00	NIST Webbook
hvapt	53.00	kJ/mol	392.00	NIST Webbook
hvapt	51.10	kJ/mol	399.00	NIST Webbook
hvapt	63.90	kJ/mol	362.50	NIST Webbook
hvapt	46.50	kJ/mol	360.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46295e+01
Coeff. B	-3.07245e+03

Coeff. C	-1.16098e+02
Temperature range (K), min.	330.33
Temperature range (K), max.	445.83

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626891&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
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

Legend

cpg:	Ideal gas 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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.