

1,5-Pentanediol

Other names:	1,5-DIHYDROXYPENTANE 1,5-PENTYLENE GLYCOL 1,5-Pentamethylene glycol 1,5-Pentandiol NSC 5927 PENTAMETHYLENE GLYCOL Pentane diol-1,5 Pentane-1,5-diol Pentylene glycol pentamethyleneglycol «alpha»,«omega»-Pentanediol Â«alphaÂ»,Â«omegaÂ»-Pentanediol
Inchi:	InChI=1S/C5H12O2/c6-4-2-1-3-5-7/h6-7H,1-5H2
InchiKey:	ALQSHHUCVQOPAS-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	OCCCCCO
Mol. weight [g/mol]:	104.15
CAS:	111-29-5

Physical Properties

Property code	Value	Unit	Source
chl	-3156.00	kJ/mol	NIST Webbook
chl	-3153.70 ± 5.70	kJ/mol	NIST Webbook
chl	-3151.10 ± 2.80	kJ/mol	NIST Webbook
gf	-282.42	kJ/mol	Joback Method
hf	-449.00 ± 3.00	kJ/mol	NIST Webbook
hf	-444.50	kJ/mol	NIST Webbook
hf	-442.00 ± 5.70	kJ/mol	NIST Webbook
hfl	-531.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-528.80 ± 5.70	kJ/mol	NIST Webbook
hfl	-526.51	kJ/mol	NIST Webbook
hfus	16.88	kJ/mol	Joback Method
hvap	86.80	kJ/mol	NIST Webbook
hvap	86.80 ± 0.50	kJ/mol	NIST Webbook
hvap	82.00	kJ/mol	NIST Webbook
hvap	86.80 ± 0.50	kJ/mol	NIST Webbook
log10ws	-0.44		Crippen Method

logp	0.141		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
pc	4362.63	kPa	Joback Method
rinpol	1016.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	993.00		NIST Webbook
sl	321.30	J/mol×K	NIST Webbook
tb	498.16	K	Joback Method
tc	731.00	K	Critical temperatures and pressures of straight-chain alkanediols (C3 to C12)
tf	378.00 ± 2.00	K	NIST Webbook
tf	257.55	K	NIST Webbook
tf	257.55 ± 0.60	K	NIST Webbook
tt	254.40 ± 0.10	K	NIST Webbook
tt	248.00 ± 0.20	K	NIST Webbook
tt	248.00 ± 0.40	K	NIST Webbook
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.03	J/mol×K	498.16	Joback Method
cpg	220.51	J/mol×K	524.48	Joback Method
cpg	227.70	J/mol×K	550.80	Joback Method
cpg	234.63	J/mol×K	577.12	Joback Method
cpg	241.29	J/mol×K	603.44	Joback Method
cpg	247.69	J/mol×K	629.76	Joback Method
cpg	253.84	J/mol×K	656.08	Joback Method
cpl	234.25	J/mol×K	300.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	236.39	J/mol×K	303.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	237.47	J/mol×K	305.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	238.56	J/mol×K	306.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	239.66	J/mol×K	308.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	240.77	J/mol×K	309.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	241.89	J/mol×K	311.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	243.01	J/mol×K	312.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	244.14	J/mol×K	314.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	245.28	J/mol×K	315.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	246.43	J/mol×K	317.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	247.59	J/mol×K	318.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	248.76	J/mol×K	320.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	249.93	J/mol×K	321.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	251.11	J/mol×K	323.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	252.30	J/mol×K	324.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	253.50	J/mol×K	326.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	254.70	J/mol×K	327.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	255.92	J/mol×K	329.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	257.14	J/mol×K	330.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	258.37	J/mol×K	332.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	259.61	J/mol×K	333.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	260.86	J/mol×K	335.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	262.11	J/mol×K	336.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	263.38	J/mol×K	338.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	264.65	J/mol×K	339.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	265.93	J/mol×K	341.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	267.22	J/mol×K	342.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	268.51	J/mol×K	344.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	269.82	J/mol×K	345.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	271.13	J/mol×K	347.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	272.45	J/mol×K	348.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	273.78	J/mol×K	350.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	275.12	J/mol×K	351.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	235.31	J/mol×K	302.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	233.19	J/mol×K	299.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	232.49	J/mol×K	298.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	232.14	J/mol×K	297.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	231.10	J/mol×K	296.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	230.06	J/mol×K	294.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	276.46	J/mol×K	353.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	229.04	J/mol×K	293.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
dvisc	0.0206552	Pa×s	306.15	Joback Method
dvisc	0.1491746	Pa×s	267.75	Joback Method
dvisc	0.0002064	Pa×s	459.76	Joback Method
dvisc	0.0004766	Pa×s	421.36	Joback Method
dvisc	0.0013011	Pa×s	382.95	Joback Method
dvisc	0.0044439	Pa×s	344.55	Joback Method
dvisc	0.0001017	Pa×s	498.16	Joback Method
hfust	15.73	kJ/mol	248.00	NIST Webbook
hfust	15.72	kJ/mol	248.00	NIST Webbook
hfust	15.72	kJ/mol	248.00	NIST Webbook
hvapt	82.00 ± 2.00	kJ/mol	446.00	NIST Webbook
hvapt	78.60	kJ/mol	435.00	NIST Webbook
hvapt	83.00	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography

rhoI	980.70	kg/m3	308.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether
rhoI	983.60	kg/m3	303.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether
rhoI	977.80	kg/m3	313.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether
rhoI	974.90	kg/m3	318.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether

rhoI	971.90	kg/m3	323.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether
rhoI	986.50	kg/m3	298.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether
rhoI	965.90	kg/m3	333.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether
rhoI	989.30	kg/m3	293.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether

rhoI	992.20	kg/m3	288.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether
rhoI	995.00	kg/m3	283.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether
rhoI	998.00	kg/m3	278.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether
rhoI	974.30	kg/m3	308.15	Molecular interactions of α , ω -alkanediols in pyrrolidin-2-one: Thermophysical and spectroscopic measurements
rhoI	974.30	kg/m3	308.15	Structural and interactional studies of homologous series of α , ω -alkanediols in N,N-dimethylformamide

rho1	969.00	kg/m3	328.15	Speed of sound and density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether
sfust	63.40	J/mol×K	248.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63841e+01
Coeff. B	-5.04129e+03
Coeff. C	-8.35280e+01
Temperature range (K), min.	396.72
Temperature range (K), max.	538.82

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.31429e+01
Coeff. B	-1.16599e+04
Coeff. C	-9.12856e+00
Coeff. D	4.45506e-06
Temperature range (K), min.	257.15
Temperature range (K), max.	673.00

Sources

Thermodynamics of phase transfer for polar molecules from alkanes to deep eutectic solvents.

<https://www.doi.org/10.1016/j.fluid.2017.05.008>

KDB Vapor Pressure Data:

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=921>

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
Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K:	https://www.doi.org/10.1021/je800356x
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Structural and interactional studies of homologous series of a,x-alkanediols in 1,4-dioxane, pyrrolidine and critical temperatures and pressures of straight-chain alkanediols (C3 to C12):	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Molecular interactions of a,x-alkanediols in pyrrolidin-2-one: Thermodynamic and spectroscopic measurements at infinite dilution for liquid phase behavior of	https://www.doi.org/10.1016/j.jct.2006.10.004
hexafluorophosphate ionic liquids with bis(hydroxyethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2007.08.005
Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography:	https://www.doi.org/10.1016/j.jct.2014.04.024
Liquid-Liquid Equilibria in Binary Mixtures of Dihydroxy Alcohols and Small Organic Compounds: Density of water + 1,5-pentanediol mixtures in a wide temperature range. Comparison with mixtures of water with diethylene glycol, propoxyethanol and diethylene glycol dimethyl ether:	https://www.doi.org/10.1016/j.fluid.2011.11.004
	https://www.thermo.com/files/research/kdb/mol/mol921.mol
	https://www.doi.org/10.1021/je060333x
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111295&Units=SI
	https://www.doi.org/10.1021/acs.jced.9b00283
	https://www.doi.org/10.1016/j.jct.2017.06.001

Legend

chl:	Standard liquid enthalpy of combustion
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
hfust:	Enthalpy of fusion at a given temperature
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
vpap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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