1,6-Hexanediol

Other names:	.alpha.,.omega.-hexanediol
	.omega.-hexanediol
	1,6-DIHYDROXYHEXANE
	HDO
	HEXAMETHYLENE GLYCOL
	Hexamethylenediol
	Hexane-1,6-diol
	Hexanediol-(1,6)
	«alpha»,«omega»-Hexanediol
	Â«alphaÂ»,Â«omegaÂ»-Hexanediol
Inchi:	InChI=1S/C6H14O2/c7-5-3-1-2-4-6-8/h7-8H,1-6H2
InchiKey:	XXMIOPMDWAUFGU-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	OCCCCCCO
Mol. weight [g/mol]:	118.17
CAS:	629-11-8

Physical Properties

Property code	Value	Unit	Source
chs	-3791.90 ± 4.80	kJ/mol	NIST Webbook
chs	-3778.01 ± 0.60	kJ/mol	NIST Webbook
chs	-3787.70 ± 4.40	kJ/mol	NIST Webbook
chs	-3999.80 ± 2.30	kJ/mol	NIST Webbook
gf	-274.00	kJ/mol	Joback Method
hf	-461.10 ± 5.40	kJ/mol	NIST Webbook
hf	-253.40	kJ/mol	NIST Webbook
hf	-462.10 ± 4.40	kJ/mol	NIST Webbook
hf	-459.40 ± 1.90	kJ/mol	NIST Webbook
hfs	-362.17	kJ/mol	NIST Webbook
hfs	-583.86 ± 0.72	kJ/mol	NIST Webbook
hfs	-569.90 ± 5.00	kJ/mol	NIST Webbook
hfs	-574.10 ± 4.40	kJ/mol	NIST Webbook
hfus	19.47	kJ/mol	Joback Method
hvap	90.70 ± 1.10	kJ/mol	NIST Webbook
hvap	98.50 ± 1.80	kJ/mol	NIST Webbook
hvap	90.90 ± 4.10	kJ/mol	NIST Webbook
log10ws	-0.86		Crippen Method

logp	0.531		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3000.00 ± 400.00	kPa	NIST Webbook
pc	4080.00	kPa	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
rhoc	294.25 ± 15.36	kg/m3	NIST Webbook
rinpol	1114.38		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1138.00		NIST Webbook
tb	516.15 ± 3.00	K	NIST Webbook
tb	523.20	K	NIST Webbook
tc	700.00 ± 4.00	K	NIST Webbook
tc	734.00	K	Critical temperatures and pressures of straight-chain alkanediols (C3 to C12)
tf	314.70	K	Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-.alpha.,.omega.-diols HO-(CH2)n-OH: Structure-related odd even effect
tt	314.60 ± 0.20	K	NIST Webbook
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.05	J/mol×K	521.04	Joback Method
cpg	301.09	J/mol×K	678.43	Joback Method
cpg	294.16	J/mol×K	652.20	Joback Method
cpg	286.94	J/mol×K	625.97	Joback Method
cpg	279.43	J/mol×K	599.73	Joback Method
cpg	271.62	J/mol×K	573.50	Joback Method
cpg	263.49	J/mol×K	547.27	Joback Method
cpl	307.41	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	317.77	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	316.31	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	314.84	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	313.36	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	295.22	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	310.40	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	308.91	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	296.76	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	311.88	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	298.30	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	299.83	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	301.36	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	302.88	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	304.40	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	282.66	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	284.25	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	285.84	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	287.42	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	288.99	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	290.55	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	292.12	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	293.67	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	305.91	J/mol×K	341.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cps	202.90	J/mol×K	298.15	NIST Webbook
dvisc	0.0145873	Pa×s	319.36	Joback Method
dvisc	0.0032062	Pa×s	359.69	Joback Method
dvisc	0.0009565	Pa×s	400.03	Joback Method
dvisc	0.0003562	Pa×s	440.37	Joback Method
dvisc	0.0001565	Pa×s	480.70	Joback Method
dvisc	0.0000781	Pa×s	521.04	Joback Method
dvisc	0.1028495	Pa×s	279.02	Joback Method
hfust	22.60	kJ/mol	315.00	NIST Webbook
hfust	25.52	kJ/mol	320.60	NIST Webbook
hfust	25.50	kJ/mol	316.00	NIST Webbook
hfust	25.52	kJ/mol	340.60	NIST Webbook
hfust	25.52	kJ/mol	320.60	NIST Webbook
hvapt	87.80 ± 1.10	kJ/mol	457.00	NIST Webbook
hvapt	73.90 ± 0.70	kJ/mol	457.00	NIST Webbook
hvapt	80.80 ± 0.90	kJ/mol	457.00	NIST Webbook
hvapt	67.00 ± 0.60	kJ/mol	457.00	NIST Webbook
hvapt	90.20	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography
hvapt	87.00	kJ/mol	342.00	NIST Webbook
pvap	10.00	kPa	456.93	Isobaric Vapor-Liquid Equilibrium for the Binary System of Dimethyl Adipate and 1,6-Hexanediol at 10, 20, and 99 kPa

pvap	20.00	kPa	474.79	Isobaric Vapor-Liquid Equilibrium for the Binary System of Dimethyl Adipate and 1,6-Hexanediol at 10, 20, and 99 kPa
pvap	99.00	kPa	525.10	Isobaric Vapor-Liquid Equilibrium for the Binary System of Dimethyl Adipate and 1,6-Hexanediol at 10, 20, and 99 kPa
sfust	79.61	J/mol×K	320.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63604e+01
Coeff. B	-5.12658e+03
Coeff. C	-8.66000e+01
Temperature range (K), min.	405.56
Temperature range (K), max.	550.59

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.72529e+01
Coeff. B	-1.09851e+04
Coeff. C	-3.34294e+00
Coeff. D	-2.05207e-06
Temperature range (K), min.	315.15
Temperature range (K), max.	670.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
293.15	101.13	947.0

Reference *https://www.doi.org/10.1021/acs.jced.9b00134*

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Effect of temperature on the surface tension of diluted aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol and 2,5-hexanediol:	https://www.doi.org/10.1016/j.fluid.2007.05.029
Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-alpha,omega-diols	https://www.doi.org/10.1016/j.jct.2013.08.019
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
HO-CnH2n-OH: Structure-related odd even effect:	https://www.doi.org/10.1021/acs.jced.9b00134
Thermophysical and Molar Volume Aberration of Amphiphilic Eutectic Mix of Branched Diols and Ammonium Ionic Liquid:	https://www.doi.org/10.1021/acs.jced.9b00306
Isobaric Vapour-Liquid Equilibrium for the Binary System of Dimethyl Adipate and 1,6-Hexanediol at 10, 20, and 99 kPa:	https://www.doi.org/10.1021/je0602465
Critical Point and Vapor Pressure Measurements for Four Compounds by a Low-Residence Time Flow Method:	https://www.doi.org/10.1021/je800356x
Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	https://www.doi.org/10.1021/je060333x
Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography:	https://www.doi.org/10.1021/acs.jced.8b00600
Activity Coefficients at Infinite Dilution of Various Solutes in Tetrapropylammonium Bromide + 1,6-Hexanediol Deep Eutectic Solvent:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=923
KDB Vapor Pressure Data:	https://www.doi.org/10.1016/j.jct.2007.01.009
Effect of temperature on the volumetric properties of dilute aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol, and 2,5-hexanediol:	https://www.cheric.org/files/research/kdb/mol/mol923.mol
KDB:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629118&Units=SI
NIST Webbook:	https://www.doi.org/10.1016/j.fluid.2013.06.048
Critical temperatures and pressures of straight-chain alkanediols (C3 to C12):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=923
KDB Pure (Korean Thermophysical Properties Databank):	https://en.wikipedia.org/wiki/Joback_method
Joback Method:	

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid 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
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume