1,2-Hexanediol

Other names: DL-hexane-1,2-diol
Inchi: InChI=1S/C6H14O2/c1-2-3-4-6(8)5-7/h6-8H,2-5H2,1H3
InchiKey: FHKSXSQHXQEMOK-UHFFFAOYSA-N
Formula: C6H14O2
SMILES: CCCCC(O)CO
Mol. weight [g/mol]: 118.17
CAS: 6920-22-5

Physical Properties

Property code	Value	Unit	Source
chl	-3784.80 ± 7.10	kJ/mol	NIST Webbook
gf	-276.44	kJ/mol	Joback Method
hf	-490.10 ± 7.10	kJ/mol	NIST Webbook
hfl	-577.10 ± 7.10	kJ/mol	NIST Webbook
hfus	15.95	kJ/mol	Joback Method
hvap	78.70 ± 0.30	kJ/mol	NIST Webbook
hvap	87.00 ± 0.30	kJ/mol	NIST Webbook
hvap	87.00	kJ/mol	NIST Webbook
log10ws	-0.97		Crippen Method
logp	0.530		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
rinpol	1145.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1147.00		NIST Webbook
tb	496.65 ± 4.00	K	NIST Webbook

tb	496.70	K	NIST Webbook
tc	680.76	K	Joback Method
tf	264.02	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.99	J/mol×K	627.37	Joback Method
cpg	272.33	J/mol×K	573.99	Joback Method
cpg	264.02	J/mol×K	547.29	Joback Method
cpg	255.37	J/mol×K	520.60	Joback Method
cpg	295.34	J/mol×K	654.07	Joback Method
cpg	302.40	J/mol×K	680.76	Joback Method
cpg	280.32	J/mol×K	600.68	Joback Method
dvisc	0.0241200	Pa×s	313.15	Excess molar volume and viscosity deviation for binary mixtures of polyethylene glycol dimethyl ether 250 with 1,2-alkanediols (C3 C6) at T = (293.15 to 323.15) K
dvisc	0.0147900	Pa×s	323.15	Excess molar volume and viscosity deviation for binary mixtures of polyethylene glycol dimethyl ether 250 with 1,2-alkanediols (C3 C6) at T = (293.15 to 323.15) K
dvisc	0.0834100	Pa×s	293.15	Excess molar volume and viscosity deviation for binary mixtures of polyethylene glycol dimethyl ether 250 with 1,2-alkanediols (C3 C6) at T = (293.15 to 323.15) K

dvisc	0.0422500	Pa×s	303.15	Excess molar volume and viscosity deviation for binary mixtures of polyethylene glycol dimethyl ether 250 with 1,2-alkanediols (C3 C6) at T = (293.15 to 323.15) K
rhol	951.68	kg/m3	293.15	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
rhol	955.23	kg/m3	288.15	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
rhol	944.54	kg/m3	303.15	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
rhol	948.08	kg/m3	298.15	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

rhol	958.87	kg/m3	283.15	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	
rhol	937.06	kg/m3	313.15	Excess volumes and excess heat capacities for alkanediol + water systems in the temperature interval (283.15-313.15) K	
rhol	944.44	kg/m3	303.15	Excess volumes and excess heat capacities for alkanediol + water systems in the temperature interval (283.15-313.15) K	
rhol	948.10	kg/m3	298.15	Excess volumes and excess heat capacities for alkanediol + water systems in the temperature interval (283.15-313.15) K	
rhol	951.73	kg/m3	293.15	Excess volumes and excess heat capacities for alkanediol + water systems in the temperature interval (283.15-313.15) K	
rhol	940.88	kg/m3	308.15	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	

rhol	958.85	kg/m3	283.15	Excess volumes and excess heat capacities for alkanediol + water systems in the temperature interval (283.15-313.15) K	
srf	0.02	N/m	308.15	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	
srf	0.02	N/m	303.15	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	
srf	0.02	N/m	293.15	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	
srf	0.02	N/m	288.15	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	
srf	0.02	N/m	283.15	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	

srf	0.02	N/m	298.15	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66265e+01
Coeff. B	-4.98928e+03
Coeff. C	-7.93580e+01
Temperature range (K), min.	384.72
Temperature range (K), max.	520.30

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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: systems the temperature interval (283.15-313.15) K:	https://www.doi.org/10.1016/j.jct.2007.01.009
Excess volumes and excess heat capacities for alkanediol + water systems at temperature	https://www.doi.org/10.1016/j.fluid.2013.06.041
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
Phase behavior of imidazolium and phosphonium tetrafluoroborates with dihydroxy alcohols:	https://www.doi.org/10.1016/j.fluid.2014.08.028
Liquid phase behavior of hexafluorophosphate ionic liquids with polyhydroxy alcohols:	https://www.doi.org/10.1016/j.fluid.2011.11.004
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic Properties of Mixtures Containing Ionic Liquids.4.LLE of Binary Mixtures of [C2MIM][NTf2] with 1-Pentanol, 1-Butanol, 1-Hexanol, and 1-Heptanol	https://www.doi.org/10.1021/je049564z
Solubility, comparison and partial molar volumes of 1,2-hexanediol before and after micellization	https://www.doi.org/10.1016/j.jct.2012.08.020
Crippen Method modification by methyl Pentan-1-ol and [C4MIM][NTf2] with	http://pubs.acs.org/doi/abs/10.1021/ci990307l
oxalyl chloride and diethyl oxalyl	
Cyclohexanol and 1,2- Hexanediol	
NIST Webbook:	http://webbook.nist.org/cgi/cbook.cgi?ID=C6920225&Units=SI
including Studies of the Influence of supercritical CO2:	
Small Amounts of Water:	
Excess molar volume and viscosity deviation for binary mixtures of polyethylene glycol dimethyl ether 250 with 1,2-alkanediols (C3 C6) at T = (293.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2008.01.022

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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