Hexylene glycol

Other names:	(.+/-.)-2-Methyl-2,4-pentanediol
	1,1,3-Trimethyltrimethylenediol
	2,4-Dihydroxy-2-methylpentane
	2,4-Pentanediol, 2-methyl-
	2-Methyl pentane-2,4-diol
	2-Methyl-2,4-pentandiol
	2-Methyl-2,4-pentanediol
	2-Methylpentan-2,4-diol
	4-Methyl-2,4-pentanediol
	4-Methyl-2,4-pentanediole
	DL-2-methyl-2,4-pentanediol
	Diolane
	Isol
	Isophthalic acid
	NSC 8098
	Pinakon
	diacetone glycol
	«alpha»,«alpha»,«alpha»'-Trimethyltrimethylene glycol
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»'-Trimethyltrimethylene glycol
Inchi:	InChI=1S/C6H14O2/c1-5(7)4-6(2,3)8/h5,7-8H,4H2,1-3H3/t5-/m0/s1
InchiKey:	SVTBMSDMJJWYQN-YFKPBYRVSA-N
Formula:	C6H14O2
SMILES:	CC(O)CC(C)(C)O
Mol. weight [g/mol]:	118.17
CAS:	107-41-5

Physical Properties

Property code	Value	Unit	Source
gf	-273.60	kJ/mol	Joback Method
hf	-485.66	kJ/mol	Joback Method
hfus	8.53	kJ/mol	Joback Method
hvap	68.60 ± 0.40	kJ/mol	NIST Webbook
hvap	68.90 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.08		Crippen Method
logp	0.528		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method

rinpol	898.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	898.00		NIST Webbook
ripol	1637.00		NIST Webbook
ripol	1637.00		NIST Webbook
tb	469.15 ± 1.00	K	NIST Webbook
tb	470.25 ± 1.00	K	NIST Webbook
tb	470.15	K	NIST Webbook
tb	471.20	K	NIST Webbook
tb	471.42 ± 0.50	K	NIST Webbook
tc	685.89	K	Joback Method
tf	266.44	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.90	J/mol×K	517.37	Joback Method
cpg	268.16	J/mol×K	545.46	Joback Method
cpg	276.95	J/mol×K	573.54	Joback Method
cpg	285.31	J/mol×K	601.63	Joback Method
cpg	293.24	J/mol×K	629.72	Joback Method
cpg	300.78	J/mol×K	657.80	Joback Method
cpg	307.94	J/mol×K	685.89	Joback Method
cpl	271.31	J/mol×K	308.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	267.10	J/mol×K	303.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature

cpl	263.09	J/mol×K	298.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	275.53	J/mol×K	313.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	279.94	J/mol×K	318.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	284.50	J/mol×K	323.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	289.17	J/mol×K	328.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	293.90	J/mol×K	333.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature

cpl	298.68	J/mol×K	338.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	303.35	J/mol×K	343.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	313.68	J/mol×K	353.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
dvisc	0.0000728	Pa×s	517.37	Joback Method
dvisc	0.0300065	Pa×s	308.26	Joback Method
dvisc	0.0050606	Pa×s	350.08	Joback Method
dvisc	0.0012479	Pa×s	391.90	Joback Method
dvisc	0.3110979	Pa×s	266.44	Joback Method
dvisc	0.0001588	Pa×s	475.55	Joback Method
dvisc	0.0004031	Pa×s	433.73	Joback Method
hvapt	58.10	kJ/mol	423.00	NIST Webbook
pvap	0.03	kPa	309.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	3.33e-03	kPa	287.90	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	4.74e-03	kPa	291.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	6.48e-03	kPa	294.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols

pvap	8.58e-03	kPa	297.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.01	kPa	300.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.01	kPa	303.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.12	kPa	329.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	2.50e-03	kPa	285.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.03	kPa	312.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.04	kPa	315.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.05	kPa	318.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.06	kPa	321.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.08	kPa	323.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.09	kPa	326.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.02	kPa	306.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols

rfi	1.42580		298.15	Study of the Effects of Temperature and Pressure on the Acoustic and Thermodynamic Properties of 2-Methyl-2,4-pentanediol
rhol	915.60	kg/m3	298.15	Isobaric Vapor Liquid Equilibrium for Two Binary Systems, (3-Methyl-1-butanol + 1,4-Butanediol) and (Hexylene Glycol + 1,4-Butanediol), at p = 40.0, 60.0, and 80.0 kPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.00693e+02
Coeff. B	-1.74091e+04
Coeff. C	-2.62395e+01
Coeff. D	1.11703e-05
Temperature range (K), min.	223.15
Temperature range (K), max.	621.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isobaric Vapor Liquid Equilibrium for Two Binary Systems, (3-Methyl-1-butanol + 1,4-Butanediol) and (Hexylene Glycol + 1,4-Butanediol), at p = 40.0, 60.0, and 80.0 kPa:	https://www.doi.org/10.1021/acs.jced.6b00092
Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,2-Butanediols:	https://www.doi.org/10.1021/je060419q
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=924
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=924
Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature:	https://www.doi.org/10.1016/j.jct.2007.04.011
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107415&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Study of the Effects of Temperature and Pressure on the Acoustic and Thermodynamic Properties of 2-Methyl-2,4-pentanediol: https://www.doi.org/10.1021/je800244q

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
pvap:	Vapor pressure
rfi:	Refractive Index
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