Neopentyl glycol

Other names:	1,3-Dihydroxy-2,2-dimethylpropane
	1,3-Propanediol, 2,2-dimethyl-
	2,2-Dimethyl-1,3-dihydroxypropane
	2,2-Dimethyl-1,3-propanediol
	2,2-Dimethylpropane-1,3-diol
	2,2-Dimethyltrimethylene glycol
	Dimethylolpropane
	Dimethyltrimethylene glycol
	Hydroxypivalyl alcohol
	NPG
	NPG Glycol
	NSC 55836
	Neol
	Neopentanediol
	Neopentylene glycol
Inchi:	InChI=1S/C5H12O2/c1-5(2,3-6)4-7/h6-7H,3-4H2,1-2H3
InchiKey:	SLCVBVWXLSEKPL-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	CC(C)(CO)CO
Mol. weight [g/mol]:	104.15
CAS:	126-30-7

Physical Properties

Property code	Value	Unit	Source
chs	-3131.30 ± 4.30	kJ/mol	NIST Webbook
gf	-279.58	kJ/mol	Joback Method
hf	-459.74	kJ/mol	Joback Method
hfs	-551.00 ± 4.20	kJ/mol	NIST Webbook
hfus	12.24	kJ/mol	Heat capacity measurement of organic thermal energy storage materials
hvap	58.79	kJ/mol	Joback Method
log10ws	-0.20		Crippen Method
logp	-0.003		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	4474.22	kPa	Joback Method
rinpol	895.00		NIST Webbook

tb	473.00 ± 2.00	K	NIST Webbook
tb	475.65 ± 4.00	K	NIST Webbook
tb	478.95	K	Investigation on Thermodynamics in Separation for Ethylene Glycol + Neopentyl Glycol System by Azeotropic Distillation
tc	687.00	K	Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method
tf	400.00 ± 3.00	K	NIST Webbook
tf	400.50 ± 1.50	K	NIST Webbook
tf	403.00 ± 3.00	K	NIST Webbook
tf	398.70 ± 2.00	K	NIST Webbook
tf	403.00 ± 1.50	K	NIST Webbook
tt	403.30 ± 0.10	K	NIST Webbook
tt	314.95	K	Phase transition of neopentyl glycol in nanopores for thermal energy storage
vc	0.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.18	J/mol×K	633.61	Joback Method
cpg	239.64	J/mol×K	578.14	Joback Method
cpg	246.59	J/mol×K	605.87	Joback Method
cpg	216.54	J/mol×K	494.93	Joback Method
cpg	259.45	J/mol×K	661.34	Joback Method
cpg	232.33	J/mol×K	550.40	Joback Method
cpg	224.63	J/mol×K	522.67	Joback Method
cps	183.18	J/mol×K	298.15	NIST Webbook
cps	183.18	J/mol×K	298.15	NIST Webbook
dvisc	0.0005115	Pa×s	420.01	Joback Method
dvisc	0.0247700	Pa×s	307.63	Joback Method
dvisc	0.0001025	Pa×s	494.93	Joback Method
dvisc	0.0002144	Pa×s	457.47	Joback Method
dvisc	0.1849815	Pa×s	270.17	Joback Method
dvisc	0.0014473	Pa×s	382.55	Joback Method
dvisc	0.0051321	Pa×s	345.09	Joback Method
hfust	4.55	kJ/mol	401.20	NIST Webbook
hfust	7.52	kJ/mol	244.00	NIST Webbook

hfust	4.23	kJ/mol	401.60	NIST Webbook
hfust	4.34	kJ/mol	402.80	NIST Webbook
hfust	4.30	kJ/mol	402.50	NIST Webbook
hfust	4.60	kJ/mol	403.20	NIST Webbook
hfust	4.60	kJ/mol	403.20	NIST Webbook
hfust	13.80	kJ/mol	315.20	NIST Webbook
hvapt	79.40	kJ/mol	440.00	NIST Webbook
psub	0.02	kPa	320.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.02	kPa	323.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.01	kPa	317.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.03	kPa	326.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.05	kPa	332.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.07	kPa	335.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.08	kPa	338.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.11	kPa	341.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.13	kPa	344.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.17	kPa	347.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols

psub	0.04	kPa	329.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.01	kPa	314.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	101.30	kPa	478.95	Investigation on Thermodynamics in Separation for Ethylene Glycol + Neopentyl Glycol System by Azeotropic Distillation
sfust	11.41	J/mol×K	403.20	NIST Webbook
sfust	43.78	J/mol×K	315.20	NIST Webbook
tconds	0.32	W/m×K	363.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys
tconds	0.31	W/m×K	393.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys
tconds	0.33	W/m×K	353.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys
tconds	0.36	W/m×K	343.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys

tconds	0.38	W/m×K	333.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys
tconds	0.40	W/m×K	323.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys
tconds	0.30	W/m×K	383.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys
tconds	0.29	W/m×K	373.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.32555e+02
Coeff. B	-1.93531e+04
Coeff. C	-3.09511e+01
Coeff. D	1.45892e-05
Temperature range (K), min.	400.00
Temperature range (K), max.	643.00

Sources

Phase Behavior of 2,2-Dimethyl-1,3-propanediol in Carbon Dioxide:	https://www.doi.org/10.1021/je8001514
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=922
Kyung-Kyu:	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys:	https://www.doi.org/10.1016/j.tca.2011.12.021
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Phase transition of neopentyl glycol in nanopores for thermal energy storage:	https://www.doi.org/10.1016/j.tca.2016.03.016
Partial Molar Isentropic Compressions and Partial Molar Volumes of Selected Branched Aliphatic Alcohols at Infinite Dilution in Water at Temperatures from T = (278 to 318) K and Atmospheric Pressure:	https://www.doi.org/10.1021/je300175w
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol922.mol
Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method:	https://www.doi.org/10.1016/j.fluid.2014.07.038
Investigation on Thermodynamics in Separation for Ethylene Glycol + Neopentyl Glycol System by Azeotropic Distillation:	https://www.doi.org/10.1021/acs.jced.5b01044
Heat capacity measurement of organic thermal energy storage materials:	https://www.doi.org/10.1016/j.jct.2006.02.005
Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols:	https://www.doi.org/10.1021/je060419q
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126307&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature

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