

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 Neopentenediol 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	478.95	K	Investigation on Thermodynamics in Separation for Ethylene Glycol + Neopentyl Glycol System by Azeotropic Distillation
tb	475.65 ± 4.00	K	NIST Webbook
tb	473.00 ± 2.00	K	NIST Webbook
tc	687.00	K	Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method
tf	403.00 ± 1.50	K	NIST Webbook
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
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.18	J/mol×K	633.61	Joback Method
cpg	216.54	J/mol×K	494.93	Joback Method
cpg	224.63	J/mol×K	522.67	Joback Method
cpg	232.33	J/mol×K	550.40	Joback Method
cpg	239.64	J/mol×K	578.14	Joback Method
cpg	246.59	J/mol×K	605.87	Joback Method
cpg	259.45	J/mol×K	661.34	Joback Method
cps	183.18	J/mol×K	298.15	NIST Webbook
cps	183.18	J/mol×K	298.15	NIST Webbook
dvisc	0.0001025	Paxs	494.93	Joback Method
dvisc	0.0014473	Paxs	382.55	Joback Method
dvisc	0.1849815	Paxs	270.17	Joback Method
dvisc	0.0005115	Paxs	420.01	Joback Method
dvisc	0.0051321	Paxs	345.09	Joback Method
dvisc	0.0002144	Paxs	457.47	Joback Method
dvisc	0.0247700	Paxs	307.63	Joback Method
hfust	4.30	kJ/mol	402.50	NIST Webbook
hfust	4.60	kJ/mol	403.20	NIST Webbook

hfust	4.55	kJ/mol	401.20	NIST Webbook
hfust	7.52	kJ/mol	244.00	NIST Webbook
hfust	4.34	kJ/mol	402.80	NIST Webbook
hfust	4.23	kJ/mol	401.60	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	0.04	kPa	329.40	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	0.07	kPa	335.30	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	0.13	kPa	344.20	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	0.02	kPa	323.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
psub	0.02	kPa	320.20	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	0.01	kPa	314.30	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	0.08	kPa	338.20	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	0.31	W/m×K	393.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys
tconds	0.40	W/m×K	323.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys
tconds	0.36	W/m×K	343.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys
tconds	0.33	W/m×K	353.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys

tconds	0.32	W/m×K	363.00	Dependency of thermal conductivity on the temperature and composition of d-camphor in the neopentylglycol d-camphor alloys
tconds	0.29	W/m×K	373.00	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	0.38	W/m×K	333.00	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	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126307&Units=SI
Investigation on Thermodynamics in Separation for Ethylene Glycol + Neopentyl Glycol System by Azeotropic Distillation:	https://www.doi.org/10.1021/acs.jced.5b01044
Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method:	https://www.chemeo.com/doc/models/crippen_log10ws https://www.doi.org/10.1016/j.fluid.2014.07.038 https://www.cheric.org/files/research/kdb/mol/mol922.mol
Heat capacity measurement of organic thermal energy storage materials: KDB Vapor Pressure Data:	https://www.doi.org/10.1016/j.jct.2006.02.005 https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=922
Phase transition of neopentyl glycol in nanopores for thermal energy storage: Dependency of thermal conductivity on the temperature and composition of the fluid:	https://www.doi.org/10.1016/j.tca.2016.03.016 https://www.doi.org/10.1016/j.tca.2011.12.021
Partial Molar Heat Capacities, Compressions and Partial Molar Volumes of Selected Branched Aliphatic Alcohols at Infinite Dilution:	https://www.doi.org/10.1021/je300175w
2,2-Dimethyl-1,3-propanediol in Carbon Dioxide: Vapor Pressure and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols:	https://www.doi.org/10.1021/je8001514 https://www.doi.org/10.1021/je060419q

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

Latest version available from:

<https://www.chemeo.com/cid/55-148-7/Neopentyl-glycol.pdf>

Generated by Cheméo on 2024-04-09 23:23:09.253302767 +0000 UTC m=+14994238.173880080.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.