1,2-Pentanediol

Other names: pentane-1,2-diol
Inchi: InChI=1S/C5H12O2/c1-2-3-5(7)4-6/h5-7H,2-4H2,1H3
InchiKey: WCVRQHFDJLLWFE-UHFFFAOYSA-N
Formula: C5H12O2
SMILES: CCCC(O)CO
Mol. weight [g/mol]: 104.15
CAS: 5343-92-0

Physical Properties

Property code	Value	Unit	Source
chl	-3135.80 ± 7.50	kJ/mol	NIST Webbook
gf	-284.86	kJ/mol	Joback Method
hf	-465.10 ± 7.50	kJ/mol	NIST Webbook
hfl	-546.70 ± 7.50	kJ/mol	NIST Webbook
hfus	13.36	kJ/mol	Joback Method
hvap	81.60 ± 0.20	kJ/mol	NIST Webbook
hvap	74.60 ± 0.30	kJ/mol	NIST Webbook
hvap	81.60	kJ/mol	NIST Webbook
log10ws	-0.55		Crippen Method
logp	0.140		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	497.72	K	Joback Method
tc	658.58	K	Joback Method
tf	252.75	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.82	J/mol×K	631.77	Joback Method
cpg	213.31	J/mol×K	497.72	Joback Method
cpg	220.99	J/mol×K	524.53	Joback Method
cpg	228.37	J/mol×K	551.34	Joback Method

cpg	235.47	J/mol×K	578.15	Joback Method
cpg	242.28	J/mol×K	604.96	Joback Method
cpg	255.10	J/mol×K	658.58	Joback Method
dvisc	0.0769600	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	0.0391600	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
dvisc	0.0225200	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	0.0136600	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
rhol	966.68	kg/m3	298.15	Excess volumes and excess heat capacities of {1,2- alkanediol + methanol} mixtures and ionic volumes in these systems

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66293e+01
Coeff. B	-4.86217e+03
Coeff. C	-7.51880e+01
Temperature range (K), min.	372.72
Temperature range (K), max.	504.79

Sources

Excess volumes and excess heat capacities of {1,2- alkanediol + methanol} mixtures and ionic volumes in these systems:	https://www.doi.org/10.1016/j.fluid.2015.05.016
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Phase behavior of imidazolium and phosphonium tetrafluoroborates with dihydroxy alcohols:	https://www.doi.org/10.1016/j.fluid.2014.08.028
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5343920&Units=SI
Liquid phase behavior of hexafluorophosphate ionic liquids with polyhydric alcohols:	https://www.doi.org/10.1016/j.fluid.2011.11.004

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume