DL-2,4-pentanediol

Other names:	(2R,4R)-2,4-pentanediol
	(R,R)-2,4-pentanediol
	2,4-Amylene glycol
	2,4-Pentanediol (dl+meso)
	2,4-pentanediol
	Isoamylene alcohol
	Pentane-2,4-diol
	Pentanediol-2,4
	[R-(R*,R*)]-2,4-pentanediol
Inchi:	InChI=1S/C5H12O2/c1-4(6)3-5(2)7/h4-7H,3H2,1-2H3
InchiKey:	GTCCGKPBSJZVRZ-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	CC(O)CC(C)O
Mol. weight [g/mol]:	104.15
CAS:	1825-14-5

Physical Properties

Property code	Value	Unit	Source
af	0.6500		Cheméo Relay (1.0)
gf	-287.30	kJ/mol	Joback Method
hf	-501.29	kJ/mol	Cheméo Relay (1.0)
hfus	9.84	kJ/mol	Joback Method
hvap	72.84	kJ/mol	Cheméo Relay (1.0)
ie	9.81	eV	Cheméo Relay (1.0)
log10ws	0.21		Cheméo Relay (1.0)
logp	0.138		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	467.74	K	Cheméo Relay (1.0)
tc	604.20	K	Cheméo Relay (1.0)
tf	279.74	K	Cheméo Relay (1.0)
vc	0.359	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.59	J/mol×K	497.28	Joback Method
cpg	221.48	J/mol×K	524.60	Joback Method
cpg	229.06	J/mol×K	551.92	Joback Method
cpg	236.33	J/mol×K	579.24	Joback Method
cpg	243.30	J/mol×K	606.56	Joback Method
cpg	249.98	J/mol×K	633.88	Joback Method
cpg	256.38	J/mol×K	661.20	Joback Method
dvisc	1.1462269	Pa×s	237.75	Joback Method
dvisc	0.0710068	Pa×s	281.00	Joback Method
dvisc	0.0092386	Pa×s	324.26	Joback Method
dvisc	0.0019427	Pa×s	367.51	Joback Method
dvisc	0.0005673	Pa×s	410.77	Joback Method
dvisc	0.0002095	Pa×s	454.02	Joback Method
dvisc	0.0000920	Pa×s	497.28	Joback Method
pvap	4.80e-03	kPa	297.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	6.45e-03	kPa	300.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	8.50e-03	kPa	303.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.01	kPa	306.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.01	kPa	309.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.02	kPa	312.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols

pvap	0.02	kPa	315.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.03	kPa	318.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.04	kPa	321.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.06	kPa	324.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.07	kPa	327.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.09	kPa	330.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.11	kPa	333.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.14	kPa	336.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.16	kPa	339.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.24	kPa	344.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.29	kPa	347.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64031e+01
Coeff. B	-4.70108e+03
Coeff. C	-7.20880e+01
Temperature range (K), min.	363.80
Temperature range (K), max.	495.93

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	
Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols:	https://www.doi.org/10.1021/je060419q
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1825145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Enthalpic Pairwise Interactions of Isomers of 2,4-pentanediol and 2,5-hexanediol in Dimethylsulfoxide + Water Mixtures at 298.15 K:	https://www.doi.org/10.1016/j.tca.2012.02.004

Legend

af:	Acentric Factor
cpg:	Ideal gas 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume