2,5-Hexanediol

Other names:	(2R,5R)-2,5-hexanediol
	2,5-Dihydroxyhexane
	Diisopropanol
	Hexan-2,5-diol
	[R-(R*,R*)]-2,5-hexanediol
	hexane-2,5-diol
Inchi:	InChI=1S/C6H14O2/c1-5(7)3-4-6(2)8/h5-8H,3-4H2,1-2H3
InchiKey:	OHMBHFSEKCCCBW-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CC(O)CCC(C)O
Mol. weight [g/mol]:	118.17
CAS:	2935-44-6

Physical Properties

Property code	Value	Unit	Source
gf	-278.88	kJ/mol	Joback Method
hf	-482.19	kJ/mol	Joback Method
hfus	12.43	kJ/mol	Joback Method
hvap	61.53	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	0.528		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	907.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	942.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		NIST Webbook
tb	480.15 ± 3.00	K	NIST Webbook
tb	493.95 ± 2.00	K	NIST Webbook
tb	363.15 ± 1.00	K	NIST Webbook
tb	490.20	K	NIST Webbook
tc	683.21	K	Joback Method
tf	249.02	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.74	J/mol×K	683.21	Joback Method
cpg	264.55	J/mol×K	547.34	Joback Method
cpg	273.06	J/mol×K	574.51	Joback Method
cpg	281.23	J/mol×K	601.69	Joback Method
cpg	289.05	J/mol×K	628.86	Joback Method
cpg	296.56	J/mol×K	656.04	Joback Method
cpg	255.68	J/mol×K	520.16	Joback Method
dvisc	0.0004135	Pa×s	429.78	Joback Method
dvisc	0.0013734	Pa×s	384.59	Joback Method
dvisc	0.0062787	Pa×s	339.40	Joback Method
dvisc	0.0457867	Pa×s	294.21	Joback Method
dvisc	0.6867154	Pa×s	249.02	Joback Method
dvisc	0.0000701	Pa×s	520.16	Joback Method
dvisc	0.0001565	Pa×s	474.97	Joback Method
rhol	968.85	kg/m3	283.15	Effect of temperature on the volumetric properties of dilute aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol, and 2,5-hexanediol
rhol	965.56	kg/m3	288.15	Effect of temperature on the volumetric properties of dilute aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol, and 2,5-hexanediol
rhol	962.17	kg/m3	293.15	Effect of temperature on the volumetric properties of dilute aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol, and 2,5-hexanediol

rhol	959.09	kg/m3	298.15	Effect of temperature on the volumetric properties of dilute aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol, and 2,5-hexanediol
rhol	955.72	kg/m3	303.15	Effect of temperature on the volumetric properties of dilute aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol, and 2,5-hexanediol
rhol	952.39	kg/m3	308.15	Effect of temperature on the volumetric properties of dilute aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol, and 2,5-hexanediol
srf	0.03	N/m	308.15	Effect of temperature on the surface tension of diluted aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol and 2,5-hexanediol
srf	0.03	N/m	303.15	Effect of temperature on the surface tension of diluted aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol and 2,5-hexanediol

srf	0.03	N/m	298.15	Effect of temperature on the surface tension of diluted aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol and 2,5-hexanediol
srf	0.03	N/m	293.15	Effect of temperature on the surface tension of diluted aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol and 2,5-hexanediol
srf	0.03	N/m	288.15	Effect of temperature on the surface tension of diluted aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol and 2,5-hexanediol
srf	0.03	N/m	283.15	Effect of temperature on the surface tension of diluted aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol and 2,5-hexanediol

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62895e+01
Coeff. B	-4.85964e+03
Coeff. C	-7.84680e+01
Temperature range (K), min.	382.16
Temperature range (K), max.	521.14

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Enthalpic Pairwise Interactions of Isomers of 2,4-pentanediol and 2,5Hexanediol in Dimethylsulfoxide + Water Mixtures at 298.15 K:	https://www.doi.org/10.1016/j.tca.2012.02.004
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Effect of temperature on the surface tension of diluted aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol, and 2,5-hexanediol:	https://www.doi.org/10.1016/j.fluid.2007.05.029
Effect of temperature on the volumetric properties of dilute aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol, and 2,5-hexanediol:	https://www.doi.org/10.1016/j.jct.2007.01.009
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2935446&Units=SI
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

Legend

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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