

1,5-Hexanediol

Other names:	hexane-1,5-diol
Inchi:	InChI=1S/C6H14O2/c1-6(8)4-2-3-5-7/h6-8H,2-5H2,1H3
InchiKey:	UNVGBIALRHLALK-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CC(O)CCCCO
Mol. weight [g/mol]:	118.17
CAS:	928-40-5

Physical Properties

Property code	Value	Unit	Source
gf	-276.44	kJ/mol	Joback Method
hf	-476.91	kJ/mol	Joback Method
hfus	15.95	kJ/mol	Joback Method
hvap	61.92	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.530		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
tb	520.60	K	Joback Method
tc	680.76	K	Joback Method
tf	264.02	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.40	J/mol×K	680.76	Joback Method
cpg	264.02	J/mol×K	547.29	Joback Method
cpg	272.33	J/mol×K	573.99	Joback Method
cpg	280.32	J/mol×K	600.68	Joback Method
cpg	287.99	J/mol×K	627.37	Joback Method
cpg	295.34	J/mol×K	654.07	Joback Method
cpg	255.37	J/mol×K	520.60	Joback Method
dvisc	0.0003828	Pa×s	435.07	Joback Method

dvisc	0.0011391	Pa×s	392.31	Joback Method
dvisc	0.0044260	Pa×s	349.55	Joback Method
dvisc	0.0251069	Pa×s	306.78	Joback Method
dvisc	0.2498961	Pa×s	264.02	Joback Method
dvisc	0.0000740	Pa×s	520.60	Joback Method
dvisc	0.0001564	Pa×s	477.84	Joback Method
rhoI	978.41	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
rhoI	975.51	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
rhoI	972.31	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
rhoI	968.91	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
rhoI	965.51	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

rhoI	962.15	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	363.20	K	0.07	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.81734e+01
Coeff. B	-5.58302e+03
Coeff. C	-8.29720e+01
Temperature range (K), min.	395.12
Temperature range (K), max.	517.05

Sources

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>

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C928405&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rho:	Liquid Density
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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