

# 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)CCCC
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	0.0001564	Paxs	477.84	Joback Method

dvisc	0.0003828	Paxs	435.07	Joback Method
dvisc	0.0011391	Paxs	392.31	Joback Method
dvisc	0.0044260	Paxs	349.55	Joback Method
dvisc	0.0251069	Paxs	306.78	Joback Method
dvisc	0.0000740	Paxs	520.60	Joback Method
dvisc	0.2498961	Paxs	264.02	Joback Method
rhol	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
rhol	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
rhol	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
rhol	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
rhol	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

rhol	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	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	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	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	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	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	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

Joback Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C928405&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C928405&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>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:</b>	<a href="https://www.doi.org/10.1016/j.fluid.2007.05.029">https://www.doi.org/10.1016/j.fluid.2007.05.029</a>
<b>Effect of temperature on the surface tension, osmotic pressure, and volumetric properties of dilute aqueous solutions of 1,2-hexanediol, 1,5-hexanediol, 1,6-hexanediol, and 2,5-hexanediol:</b>	<a href="https://www.doi.org/10.1016/j.jct.2007.01.009">https://www.doi.org/10.1016/j.jct.2007.01.009</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rhol:</b>	Liquid Density
<b>srf:</b>	Surface Tension
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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