

1,7-Heptanediol

Other names:	.alpha.,.omega.-heptanediol .omega.-heptanediol 1,7-Dihydroxyheptane Heptamethylene glycol Heptane-1,7-diol «alpha», «omega»-Heptanediol «omega»-Heptanediol Â«alphaÂ»,Â«omegaÂ»-Heptanediol Â«omegaÂ»-Heptanediol
Inchi:	InChI=1S/C7H16O2/c8-6-4-2-1-3-5-7-9/h8-9H,1-7H2
InchiKey:	SXCBDZAEHILGLM-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	OCCCCCCCO
Mol. weight [g/mol]:	132.20
CAS:	629-30-1

Physical Properties

Property code	Value	Unit	Source
chl	-4467.00 ± 9.30	kJ/mol	NIST Webbook
gf	-265.58	kJ/mol	Joback Method
hf	-477.60 ± 9.30	kJ/mol	NIST Webbook
hfl	-574.20 ± 9.30	kJ/mol	NIST Webbook
hfus	22.06	kJ/mol	Joback Method
hvap	96.60 ± 0.60	kJ/mol	NIST Webbook
hvap	96.50 ± 3.20	kJ/mol	NIST Webbook
hvap	96.20 ± 1.20	kJ/mol	NIST Webbook
hvap	96.60	kJ/mol	NIST Webbook
log10ws	-1.28		Crippen Method
logp	0.922		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	1201.00		NIST Webbook
rinpol	1201.00		NIST Webbook
tb	535.20	K	NIST Webbook
tb	532.20	K	NIST Webbook
tc	700.93	K	Joback Method
tf	293.15 ± 4.00	K	NIST Webbook

tf	337.15 ± 2.00	K	NIST Webbook
tf	290.50	K	Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-.alpha.,.omega.-diols HO-(CH2)n-OH: Structure-related odd even effect
tt	295.00 ± 0.20	K	NIST Webbook
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.33	J/molxK	596.26	Joback Method
cpg	349.86	J/molxK	700.93	Joback Method
cpg	342.22	J/molxK	674.76	Joback Method
cpg	334.25	J/molxK	648.59	Joback Method
cpg	325.96	J/molxK	622.42	Joback Method
cpg	308.35	J/molxK	570.09	Joback Method
cpg	299.02	J/molxK	543.92	Joback Method
cpl	354.42	J/molxK	353.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	342.20	J/molxK	342.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	340.50	J/molxK	341.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	338.81	J/mol×K	339.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	337.13	J/mol×K	338.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	343.91	J/mol×K	344.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	345.63	J/mol×K	345.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	335.47	J/mol×K	336.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	347.37	J/mol×K	347.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	349.11	J/mol×K	348.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	350.87	J/mol×K	350.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	352.64	J/mol×K	351.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	292.06	J/mol×K	293.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	293.40	J/mol×K	294.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	294.75	J/mol×K	296.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	296.11	J/mol×K	297.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	297.48	J/mol×K	299.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	298.87	J/mol×K	300.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	300.26	J/mol×K	302.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	301.67	J/mol×K	303.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	303.09	J/mol×K	305.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	304.51	J/mol×K	306.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	305.95	J/mol×K	308.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	332.17	J/mol×K	333.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	308.87	J/mol×K	311.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	310.34	J/mol×K	312.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	311.83	J/mol×K	314.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	313.33	J/mol×K	315.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	314.83	J/mol×K	317.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	316.35	J/mol×K	318.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	317.88	J/mol×K	320.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	319.43	J/mol×K	321.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	320.98	J/mol×K	323.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	322.54	J/mol×K	324.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	324.12	J/mol×K	326.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	325.71	J/mol×K	327.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	327.31	J/mol×K	329.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	328.00	J/mol×K	330.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K

cpl	330.54	J/molxK	332.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	307.41	J/molxK	309.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	333.81	J/molxK	335.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
dvisc	0.0001190	Paxs	501.65	Joback Method
dvisc	0.0002672	Paxs	459.38	Joback Method
dvisc	0.0007068	Paxs	417.11	Joback Method
dvisc	0.0023279	Paxs	374.83	Joback Method
dvisc	0.0103813	Paxs	332.56	Joback Method
dvisc	0.0000601	Paxs	543.92	Joback Method
dvisc	0.0715544	Paxs	290.29	Joback Method
hfust	21.30	kJ/mol	295.20	NIST Webbook
hfust	21.30	kJ/mol	295.20	NIST Webbook
hvapt	93.80	kJ/mol	323.00	NIST Webbook
hvapt	92.40	kJ/mol	341.00	NIST Webbook
hvapt	97.90	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.66473e+01
Coeff. B	-5.32013e+03
Coeff. C	-8.99220e+01

Temperature range (K), min.	415.12
Temperature range (K), max.	559.24

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamics of fusion and sublimation for a homologous series of eleven alkane- α,ω -diols	https://www.doi.org/10.1016/j.jct.2013.08.019
NIST Webbook: $\text{HO}-(\text{CH}_2)_n-\text{OH}$: Structure-related odd-even effect.	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629301&Units=SI
The Yaws Handbook of Vapor Pressure: Heat Capacities of Some Liquid α,ω -Alkanediols within the Temperature Range between (293.15 and 353.15) K:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://www.doi.org/10.1021/je800356x
Vaporization Enthalpies of the r,o -Alkanediols by Correlation Gas Chromatography:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
	https://en.wikipedia.org/wiki/Joback_method
	https://www.doi.org/10.1021/je060333x

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

vc: Critical Volume

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