1,7-HEPTANEDIOL

Other names:	.alpha.,.omega.-heptanediol
	.omega.-heptanediol
	1,7-dihydroxyheptane
	Heptamethylene glycol
	Heptane-1,7-diol
	«alpha»,«omega»-Heptanediol
	«omega»-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
af	0.8222		Cheméo Relay (1.0)
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	kJ/mol	NIST Webbook
hvap	96.20 ± 1.20	kJ/mol	NIST Webbook
hvap	96.50 ± 3.20	kJ/mol	NIST Webbook
hvap	96.60 ± 0.60	kJ/mol	NIST Webbook
ie	9.77	eV	Cheméo Relay (1.0)
log10ws	-1.37		Cheméo Relay (1.0)
logp	0.922		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	1201.00		NIST Webbook
tb	532.20	K	NIST Webbook
tb	535.20	K	NIST Webbook
tc	745.64	K	Cheméo Relay (1.0)

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
tf	337.15 ± 2.00	K	NIST Webbook
tf	293.15 ± 4.00	K	NIST Webbook
tt	295.00 ± 0.20	K	NIST Webbook
vc	0.461	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.02	J/mol×K	543.92	Joback Method
cpg	349.86	J/mol×K	700.93	Joback Method
cpg	342.22	J/mol×K	674.76	Joback Method
cpg	334.25	J/mol×K	648.59	Joback Method
cpg	325.96	J/mol×K	622.42	Joback Method
cpg	317.33	J/mol×K	596.26	Joback Method
cpg	308.35	J/mol×K	570.09	Joback Method
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	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	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	307.41	J/mol×K	309.65	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/mol×K	332.15	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	333.81	J/mol×K	335.15	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	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	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	340.50	J/mol×K	341.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
cpl	342.20	J/mol×K	342.65	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	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	354.42	J/mol×K	353.15	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	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	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
dvisc	0.0715544	Pa×s	290.29	Joback Method
dvisc	0.0103813	Pa×s	332.56	Joback Method
dvisc	0.0023279	Pa×s	374.83	Joback Method
dvisc	0.0007068	Pa×s	417.11	Joback Method
dvisc	0.0002672	Pa×s	459.38	Joback Method
dvisc	0.0001190	Pa×s	501.65	Joback Method
dvisc	0.0000601	Pa×s	543.92	Joback Method
hfust	21.30	kJ/mol	295.20	NIST Webbook
hfust	21.30	kJ/mol	295.20	NIST Webbook
hvapt	97.90	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography
hvapt	93.80	kJ/mol	323.00	NIST Webbook
hvapt	92.40	kJ/mol	341.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629301&Units=SI
Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je060333x
Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K:	https://www.doi.org/10.1021/je800356x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-alpha,omega-diols HO(CH2)nOH: Structure-related odd even effect:	https://www.doi.org/10.1016/j.jct.2013.08.019
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
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
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
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
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