1,8-Octanediol

Other names:	1,8-dihydroxyoctane
	Octamethylene glycol
	Octan-1,8-diol
	octane, 1,8-dihydroxy-
	octane-1,8-diol
Inchi:	InChI=1S/C8H18O2/c9-7-5-3-1-2-4-6-8-10/h9-10H,1-8H2
InchiKey:	OEIJHBUUFURJLI-UHFFFAOYSA-N
Formula:	C8H18O2
SMILES:	OCCCCCCCCO
Mol. weight [g/mol]:	146.23
CAS:	629-41-4

Physical Properties

Property code	Value	Unit	Source
chs	-5094.00 ± 4.80	kJ/mol	NIST Webbook
gf	-257.16	kJ/mol	Joback Method
hf	-487.30 ± 4.90	kJ/mol	NIST Webbook
hfs	-626.60 ± 4.80	kJ/mol	NIST Webbook
hfus	24.65	kJ/mol	Joback Method
hsub	139.30 ± 0.90	kJ/mol	NIST Webbook
hsub	139.30	kJ/mol	NIST Webbook
hsub	139.30 ± 0.90	kJ/mol	NIST Webbook
hvap	105.40 ± 1.80	kJ/mol	NIST Webbook
hvap	107.00 ± 2.20	kJ/mol	NIST Webbook
log10ws	-1.70		Crippen Method
logp	1.312		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1313.00		NIST Webbook
ripol	2366.00		NIST Webbook
ripol	2366.00		NIST Webbook
tb	566.80	K	Joback Method
tc	752.00	K	Critical temperatures and pressures of straight-chain alkanediols (C3 to C12)

tf	331.60	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	332.70 ± 0.10	K	NIST Webbook
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.83	J/mol×K	566.80	Joback Method
cpg	354.99	J/mol×K	592.94	Joback Method
cpg	364.75	J/mol×K	619.07	Joback Method
cpg	374.14	J/mol×K	645.21	Joback Method
cpg	383.15	J/mol×K	671.35	Joback Method
cpg	391.80	J/mol×K	697.49	Joback Method
cpg	400.10	J/mol×K	723.62	Joback Method
cpl	396.17	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	373.24	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	375.13	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	377.03	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	378.93	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	380.83	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	382.74	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	384.65	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	386.56	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	371.35	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	390.40	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	392.32	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	394.24	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	388.48	J/mol×K	347.15	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
dvisc	0.0502473	Pa×s	301.56	Joback Method
dvisc	0.0074475	Pa×s	345.77	Joback Method
dvisc	0.0017017	Pa×s	389.97	Joback Method
dvisc	0.0005252	Pa×s	434.18	Joback Method
dvisc	0.0002014	Pa×s	478.39	Joback Method
dvisc	0.0000908	Pa×s	522.59	Joback Method
dvisc	0.0000464	Pa×s	566.80	Joback Method
hfust	36.10	kJ/mol	332.80	NIST Webbook
hfust	36.10	kJ/mol	332.80	NIST Webbook
hvapt	104.90	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography
hvapt	101.00	kJ/mol	356.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	445.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.97169e+01
Coeff. B	-6.40965e+03
Coeff. C	-9.24240e+01
Temperature range (K), min.	422.32
Temperature range (K), max.	537.37

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-alpha,omega-diols	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
HCCH-CnH2n-OH: Structure-related odd even effect:	https://www.doi.org/10.1021/je800356x
Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between 293.15 and 393.15K:	https://www.doi.org/10.1016/j.fluid.2013.06.048
Critical temperatures and pressures of straight-chain alkanediols (C3 to C12):	https://en.wikipedia.org/wiki/Joback_method
Joback Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.doi.org/10.1021/je060333x
Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	https://webbook.nist.gov/cgi/cbook.cgi?ID=C629414&Units=SI
NIST Webbook:	

Legend

chs:	Standard solid 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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume