1,9-Nonanediol

Other names:	.alpha.,.omega.-nonanediol
	1,9-dihydroxynonane
	nonane-1,9-diol
	«alpha»,«OMEGA»-Nonanediol
	Â«alphaÂ»,Â«OMEGAÂ»-Nonanediol
Inchi:	InChI=1S/C9H20O2/c10-8-6-4-2-1-3-5-7-9-11/h10-11H,1-9H2
InchiKey:	ALVZNPYWJMLXKV-UHFFFAOYSA-N
Formula:	C9H20O2
SMILES:	OCCCCCCCCCO
Mol. weight [g/mol]:	160.25
CAS:	3937-56-2

Physical Properties

Property code	Value	Unit	Source
chl	-5742.30 ± 7.00	kJ/mol	NIST Webbook
gf	-248.74	kJ/mol	Joback Method
hf	-508.90 ± 7.10	kJ/mol	NIST Webbook
hfl	-657.60 ± 7.00	kJ/mol	NIST Webbook
hfus	27.24	kJ/mol	Joback Method
hvap	148.70 ± 1.10	kJ/mol	NIST Webbook
hvap	148.70	kJ/mol	NIST Webbook
hvap	112.80 ± 2.10	kJ/mol	NIST Webbook
hvap	111.40 ± 7.00	kJ/mol	NIST Webbook
log10ws	-2.12		Crippen Method
logp	1.702		Crippen Method
mcvol	149.410	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1414.00		NIST Webbook
tb	589.68	K	Joback Method
tc	760.00	K	Critical temperatures and pressures of straight-chain alkanediols (C3 to C12)
tf	318.70	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	319.50 ± 0.10	K	NIST Webbook
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.57	J/mol×K	694.28	Joback Method
cpg	451.76	J/mol×K	746.58	Joback Method
cpg	442.85	J/mol×K	720.43	Joback Method
cpg	392.38	J/mol×K	589.68	Joback Method
cpg	403.30	J/mol×K	615.83	Joback Method
cpg	413.80	J/mol×K	641.98	Joback Method
cpg	423.89	J/mol×K	668.13	Joback Method
cpl	430.82	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	436.95	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	434.92	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	432.87	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	391.15	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	393.27	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	395.39	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	397.51	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	399.62	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	401.73	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	403.84	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	405.94	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	408.03	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	410.12	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	412.21	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	414.30	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	416.38	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	418.45	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	420.52	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	422.59	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	424.66	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	426.72	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	428.77	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	389.02	J/mol×K	318.65	Heat Capacities of Some Liquid alpha,omega-Alkanediols within the Temperature Range between (293.15 and 353.15) K
dvisc	0.0001526	Pa×s	497.40	Joback Method
dvisc	0.0000696	Pa×s	543.54	Joback Method
dvisc	0.0356093	Pa×s	312.83	Joback Method
dvisc	0.0053856	Pa×s	358.97	Joback Method
dvisc	0.0012525	Pa×s	405.11	Joback Method
dvisc	0.0000359	Pa×s	589.68	Joback Method
dvisc	0.0003925	Pa×s	451.25	Joback Method
hfust	36.40	kJ/mol	319.60	NIST Webbook
hfust	36.40	kJ/mol	319.60	NIST Webbook
hvapt	112.50	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography
hvapt	104.40	kJ/mol	360.00	NIST Webbook
hvapt	110.00	kJ/mol	323.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	450.20	K	2.00	NIST Webbook
tbrp	447.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.02589e+01
Coeff. B	-6.73440e+03
Coeff. C	-9.63160e+01
Temperature range (K), min.	433.52
Temperature range (K), max.	546.86

Sources

Thermodynamics of fusion and sublimation for a homologous series of	https://www.doi.org/10.1016/j.jct.2013.08.019
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3937562&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vaporization Enthalpies of the	https://www.doi.org/10.1021/je060333x
Heat Capacities of Some Liquid	https://www.doi.org/10.1021/je800356x
Critical temperatures and pressures of	https://www.doi.org/10.1016/j.fluid.2013.06.048
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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