

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:	OCCCCCCCCO
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	kJ/mol	NIST Webbook
hvap	112.80 ± 2.10	kJ/mol	NIST Webbook
hvap	148.70 ± 1.10	kJ/mol	NIST Webbook
hvap	111.40 ± 7.00	kJ/mol	NIST Webbook
log10ws	-2.12		Crippen Method
logp	1.702		Crippen Method
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.38	J/mol×K	589.68	Joback Method
cpg	413.80	J/mol×K	641.98	Joback Method
cpg	423.89	J/mol×K	668.13	Joback Method
cpg	433.57	J/mol×K	694.28	Joback Method
cpg	442.85	J/mol×K	720.43	Joback Method
cpg	451.76	J/mol×K	746.58	Joback Method
cpg	403.30	J/mol×K	615.83	Joback Method
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	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	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	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	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	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	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	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	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	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	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	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	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	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	0.0356093	Paxs	312.83	Joback Method
dvisc	0.0053856	Paxs	358.97	Joback Method
dvisc	0.0012525	Paxs	405.11	Joback Method
dvisc	0.0003925	Paxs	451.25	Joback Method
dvisc	0.0001526	Paxs	497.40	Joback Method
dvisc	0.0000696	Paxs	543.54	Joback Method
dvisc	0.0000359	Paxs	589.68	Joback Method
hfust	36.40	kJ/mol	319.60	NIST Webbook
hfust	36.40	kJ/mol	319.60	NIST Webbook
hvapt	110.00	kJ/mol	323.00	NIST Webbook
hvapt	104.40	kJ/mol	360.00	NIST Webbook
hvapt	112.50	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography

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	$\ln(P_{vp}) = A + B/(T + C)$
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

- Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
- Thermodynamics of fusion and sublimation for a homologous series of even unbranched, 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>
- HOSEIN-OH: Structure-related odd even effect.** 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 Critical Temperatures and pressures of straight-chain alkanediols (C3 to C12):** <https://www.doi.org/10.1016/j.fluid.2013.06.048>
- McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>
- Heat Capacities of Some Liquid alpha,omega-Alkanediols within the NIST Webbook Range between (293.15 and 353.15) K:** <https://www.doi.org/10.1021/je800356x>
- <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3937562&Units=SI>

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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