1-Nonanol

Other names:	1-Hydroxynonane
	Alcohol C-9
	NSC 5521
	Nonan-1-ol
	Nonanol
	Nonanol-(1)
	Nonyl alcohol
	OCTYLCARBINOL
	Octyl carbinol
	Pelargonic alcohol
	n-Nonan-1-ol
	n-Nonanol
	n-Nonyl alcohol
Inchi:	InChI=1S/C9H20O/c1-2-3-4-5-6-7-8-9-10/h10H,2-9H2,1H3
InchiKey:	ZWRUINPWMLAQRD-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCCCCCCCO
Mol. weight [g/mol]:	144.25
CAS:	143-08-8

Physical Properties

Property code	Value	Unit	Source
chl	-5947.00 ± 1.00	kJ/mol	NIST Webbook
chl	-5939.48	kJ/mol	NIST Webbook
chl	-5939.50 ± 3.00	kJ/mol	NIST Webbook
chl	-5946.30 ± 0.60	kJ/mol	NIST Webbook
chl	-5940.80 ± 1.00	kJ/mol	NIST Webbook
dm	1.70	debye	KDB
fll	0.80	% in Air	KDB
flu	6.10	% in Air	KDB
fpc	372.04	K	KDB
fpo	347.04	K	KDB
gf	-118.30	kJ/mol	KDB
hf	-375.60 ± 2.10	kJ/mol	NIST Webbook
hf	-376.00 ± 1.30	kJ/mol	NIST Webbook
hf	-376.70 ± 1.00	kJ/mol	NIST Webbook
hf	-368.70	kJ/mol	NIST Webbook

hf	-374.30	kJ/mol	NIST Webbook
hf	-382.30 ± 1.40	kJ/mol	NIST Webbook
hf	-387.20	kJ/mol	KDB
hf	-383.50 ± 3.10	kJ/mol	NIST Webbook
hfl	-460.50 ± 3.00	kJ/mol	NIST Webbook
hfl	-459.20 ± 1.20	kJ/mol	NIST Webbook
hfl	-453.60 ± 0.60	kJ/mol	NIST Webbook
hfl	-460.40 ± 3.00	kJ/mol	NIST Webbook
hfus	23.15	kJ/mol	Joback Method
hvap	84.90	kJ/mol	NIST Webbook
hvap	74.70 ± 0.30	kJ/mol	NIST Webbook
hvap	72.20	kJ/mol	NIST Webbook
hvap	76.70	kJ/mol	NIST Webbook
hvap	77.40	kJ/mol	NIST Webbook
hvap	76.86 ± 0.75	kJ/mol	NIST Webbook
hvap	76.90 ± 0.80	kJ/mol	NIST Webbook
hvap	77.80 ± 1.90	kJ/mol	NIST Webbook
hvap	76.86	kJ/mol	NIST Webbook
log10ws	-3.01		Estimated Solubility Method
log10ws	-3.01		Aqueous Solubility Prediction Method
logp	2.729		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=1)		KDB
pc	2546.00 ± 20.00	kPa	NIST Webbook
pc	2510.00 ± 60.00	kPa	NIST Webbook
pc	2546.00 ± 20.00	kPa	NIST Webbook
pc	2528.00	kPa	KDB
pc	2530.00 ± 50.00	kPa	NIST Webbook
rhoc	252.45 ± 5.77	kg/m3	NIST Webbook
rhoc	265.43 ± 2.89	kg/m3	NIST Webbook
rhoc	263.99	kg/m3	NIST Webbook
rhoc	252.45 ± 7.21	kg/m3	NIST Webbook
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ripol	1649.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1661.00		NIST Webbook
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tb	488.20	K	NIST Webbook
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tb	486.65 ± 2.00	K	NIST Webbook
tb	486.15 ± 3.00	K	NIST Webbook
tb	486.25 ± 1.00	K	NIST Webbook
tb	486.70	K	NIST Webbook
tb	486.52	K	KDB
tb	486.45 ± 0.50	K	NIST Webbook
tb	471.55 ± 2.00	K	NIST Webbook
tc	671.00 ± 1.00	K	NIST Webbook
tc	670.40 ± 0.60	K	NIST Webbook
tc	670.40 ± 0.60	K	NIST Webbook
tc	670.50	K	NIST Webbook
tc	670.52 ± 0.70	K	NIST Webbook
tc	683.00 ± 2.00	K	NIST Webbook
tc	671.30 ± 1.00	K	NIST Webbook
tc	670.70	K	KDB
tf	267.55	K	Aqueous Solubility Prediction Method
tf	268.00	K	KDB
vc	0.572	m3/kmol	NIST Webbook
vc	0.572	m3/kmol	KDB
zc	0.2593030		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.35	J/mol×K	603.56	Joback Method
cpg	391.99	J/mol×K	630.07	Joback Method
cpg	334.38	J/mol×K	497.50	Joback Method
cpg	346.81	J/mol×K	524.01	Joback Method
cpg	358.77	J/mol×K	550.53	Joback Method
cpg	370.28	J/mol×K	577.04	Joback Method
cpg	402.22	J/mol×K	656.58	Joback Method
cpl	356.30	J/mol×K	303.10	NIST Webbook
cpl	342.90	J/mol×K	304.17	NIST Webbook
dvisc	0.0002495	Pa×s	456.58	Joback Method
dvisc	0.0001486	Pa×s	497.50	Joback Method
dvisc	0.0415724	Pa×s	252.01	Joback Method
dvisc	0.0084367	Pa×s	292.93	Joback Method
dvisc	0.0025311	Pa×s	333.84	Joback Method
dvisc	0.0009877	Pa×s	374.75	Joback Method
dvisc	0.0004639	Pa×s	415.67	Joback Method
hvapt	65.50	kJ/mol	426.00	NIST Webbook
hvapt	64.50	kJ/mol	427.50	NIST Webbook
hvapt	54.39	kJ/mol	486.60	KDB
hvapt	65.00	kJ/mol	434.00	NIST Webbook
hvapt	62.90	kJ/mol	438.00	NIST Webbook
hvapt	59.70	kJ/mol	459.50	NIST Webbook
rhol	828.00	kg/m3	293.00	KDB
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43149e+01
Coeff. B	-3.52869e+03
Coeff. C	-1.21090e+02
Temperature range (K), min.	372.65
Temperature range (K), max.	513.02

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.51000e+02
Coeff. B	-1.90455e+04
Coeff. C	-3.41120e+01
Coeff. D	1.61583e-05
Temperature range (K), min.	268.15
Temperature range (K), max.	673.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=846

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=846

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

KDB Pure (Korean Thermophysical Properties Databank): https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=846

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C143088&Units=SI

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

dm: Dipole Moment

dvisc: Dynamic viscosity

fll: Lower Flammability Limit

flu: Upper Flammability Limit

fpc: Flash Point (Closed Cup Method)

fpo: Flash Point (Open Cup Method)

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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility