

Nonanal

Other names:	1-Nonaldehyde
	1-Nonanal
	1-Nonyl aldehyde
	918959-88-3
	Aldehyde C-9
	C-9 Aldehyde
	N-NONALDEHYDE
	NCI-C61018
	NONANOIC ALDEHYDE
	NSC 5518
	Nonaldehyde
	Nonanaldehyde
	Nononal
	Nonyl aldehyde, n-
	Nonylaldehyde
	Nonylic aldehyde
	Pelargonaldehyde
	Pelargonic aldehyde
	n-Nonan-1-al
	n-Nonanal
Inchi:	InChI=1S/C9H18O/c1-2-3-4-5-6-7-8-9-10/h9H,2-8H2,1H3
InchiKey:	GYHFUZHODSMOHU-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CCCCCCCCC=O
Mol. weight [g/mol]:	142.24
CAS:	124-19-6

Physical Properties

Property code	Value	Unit	Source
af	0.5400		KDB
gf	-74.62	kJ/mol	Joback Method
hf	-314.67	kJ/mol	Joback Method
hfus	21.36	kJ/mol	Joback Method
hvap	55.20	kJ/mol	NIST Webbook
hvap	55.30 ± 0.30	kJ/mol	NIST Webbook

hvap	56.30 ± 0.20	kJ/mol	NIST Webbook
hvap	58.90	kJ/mol	NIST Webbook
log10ws	-3.17		Aqueous Solubility Prediction Method
logp	2.936		Crippen Method
mcpvol	139.240	ml/mol	McGowan Method
pc	2480.00	kPa	KDB
pc	1680.00 ± 35.00	kPa	NIST Webbook
rhoc	261.72 ± 5.69	kg/m3	NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1104.80		NIST Webbook
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tb	464.15 ± 3.00	K	NIST Webbook
tb	461.60	K	KDB
tb	458.15 ± 3.00	K	NIST Webbook
tc	658.50 ± 0.60	K	NIST Webbook
tc	640.00	K	KDB
tf	267.00	K	KDB
tf	253.83 ± 0.10	K	NIST Webbook
vc	0.556	m3/kmol	KDB
zc	0.2593580		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.25	J/mol×K	567.13	Joback Method
cpg	359.42	J/mol×K	595.41	Joback Method
cpg	298.64	J/mol×K	453.98	Joback Method
cpg	311.80	J/mol×K	482.27	Joback Method
cpg	324.45	J/mol×K	510.55	Joback Method
cpg	336.60	J/mol×K	538.84	Joback Method
cpg	370.13	J/mol×K	623.70	Joback Method
dvisc	0.0012510	Pa×s	308.15	Density and Viscosity of Several Aldehydes Fragrance Compounds in Their Binary Mixtures with Ethanol at (298.15 K, 308.15 K, and 318.15 K)
dvisc	0.0011270	Pa×s	318.15	Density and Viscosity of Several Aldehydes Fragrance Compounds in Their Binary Mixtures with Ethanol at (298.15 K, 308.15 K, and 318.15 K)

dvisc	0.0013920	Pa×s	298.15	Density and Viscosity of Several Aldehydes Fragrance Compounds in Their Binary Mixtures with Ethanol at (298.15 K, 308.15 K, and 318.15 K)
hfust	29.60	kJ/mol	253.90	NIST Webbook
hvapt	51.10	kJ/mol	382.00	NIST Webbook
hvapt	50.81	kJ/mol	461.60	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.70	K	3.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61633e+01
Coeff. B	-4.53609e+03
Coeff. C	-7.12960e+01
Temperature range (K), min.	357.02
Temperature range (K), max.	489.30

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.97569e+02
Coeff. B	-1.43661e+04
Coeff. C	-2.69986e+01
Coeff. D	1.73160e-05
Temperature range (K), min.	255.15
Temperature range (K), max.	640.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124196&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1240
Density and Viscosity of Several Aldehydes Fragrance Compounds in Subcritical CO ₂ and H ₂ O:	https://www.doi.org/10.1021/je0502344
Supercritical CO ₂ and H ₂ O Binary Mixtures with Ethanol:	https://www.doi.org/10.1021/je900148e
CO ₂ -Expanded Hydrocarbon Reaction Mixtures Containing 1-Octene and Nonanal up to 353.15 K and 9 MPa:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1240.mol

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume
zc: Critical Compressibility

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