

Decanal

Other names:	1-Decanal 1-Decyl aldehyde 1-nonanecarbaldehyde Aldehyde C10 C-10 Aldehyde CAPRALDEHYDE CAPRIC ALDEHYDE Caprinaldehyde Caprinic aldehyde Decaldehyde Decanaldehyde Decyl aldehyde Decylic aldehyde N-DECALDEHYDE NSC 6087 n-Decanal n-Decanal (capric aldehyde) n-Decyl aldehyde
Inchi:	InChI=1S/C10H20O/c1-2-3-4-5-6-7-8-9-10-11/h10H,2-9H2,1H3
InchiKey:	KSMVZQYAVGTKIV-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CCCCCCCCC=O
Mol. weight [g/mol]:	156.27
CAS:	112-31-2

Physical Properties

Property code	Value	Unit	Source
af	0.6340		KDB
gf	-66.20	kJ/mol	Joback Method
hf	-335.31	kJ/mol	Joback Method
hfus	23.95	kJ/mol	Joback Method
hvap	60.40 ± 0.30	kJ/mol	NIST Webbook
hvap	59.50 ± 0.40	kJ/mol	NIST Webbook
hvap	60.50	kJ/mol	NIST Webbook
log10ws	-3.29		Crippen Method
logp	3.326		Crippen Method
mvol	153.330	ml/mol	McGowan Method

pc	2260.00	kPa	KDB
pc	2600.00 ± 80.00	kPa	NIST Webbook
rhoc	260.96 ± 6.25	kg/m3	NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1200.00		NIST Webbook
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tb	481.60	K	KDB
tb	481.70	K	NIST Webbook
tb	479.15 ± 3.00	K	NIST Webbook
tb	481.65 ± 3.00	K	NIST Webbook
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tc	674.20 ± 1.00	K	NIST Webbook
tf	269.25 ± 0.10	K	NIST Webbook
tf	268.00	K	KDB
vc	0.613	m ³ /kmol	KDB
zc	0.2469390		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.00	J/mol×K	645.45	Joback Method
cpg	356.71	J/mol×K	504.96	Joback Method
cpg	342.64	J/mol×K	476.86	Joback Method
cpg	407.58	J/mol×K	617.36	Joback Method
cpg	395.65	J/mol×K	589.26	Joback Method
cpg	383.20	J/mol×K	561.16	Joback Method
cpg	370.23	J/mol×K	533.06	Joback Method
dvisc	0.0014120	Paxs	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	0.0012810	Paxs	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	0.0015600	Paxs	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	30.60	kJ/mol	268.20	NIST Webbook
hfust	30.60	kJ/mol	269.47	NIST Webbook
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hvapt	57.30	kJ/mol	325.50	NIST Webbook
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hvapt	56.30	kJ/mol	403.00	NIST Webbook
rhol	838.37	kg/m ³	298.20	Physical Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.2 K
sfust	113.60	J/molxK	269.47	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58013e+01
Coeff. B	-4.54602e+03
Coeff. C	-7.51880e+01
Temperature range (K), min.	368.22
Temperature range (K), max.	508.56

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.56406e+02
Coeff. B	-1.34546e+04
Coeff. C	-2.04384e+01

Coeff. D	9.95903e-06
Temperature range (K), min.	267.15
Temperature range (K), max.	657.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112312&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Quantitative NMR spectroscopy of binary liquid mixtures (aldehyde + alcohol) and Vapor Pressure of Several Aldehydes, Fragrance Compounds in 2-Butoxybenzyl Mixtures with Ethanol at 298.15 K, 308.15 K, and 318.15 K): KDB Vapor Pressure Data:	https://www.doi.org/10.1016/j.jct.2014.01.027 https://www.doi.org/10.1021/je0502344 https://www.cheric.org/files/research/kdb/mol/mol1241.mol https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1241
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure: Physical Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.2 K:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure https://www.doi.org/10.1021/acs.jced.8b00086

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
rhoL:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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