

# Octanal

<b>Other names:</b>	1-Octanal 1-heptanecarbaldehyde Aldehyde C-8 Antifoam-LF C-8 Aldehyde Caprylaldehyde Caprylic aldehyde N-CAPRYLALDEHYDE N-OCTALDEHYDE NSC 1508 Octaldehyde Octanaldehyde Octanoic aldehyde Octylaldehyde n-Octanal n-Octyl aldehyde n-Octylal octyl aldehyde
<b>Inchi:</b>	InChI=1S/C8H16O/c1-2-3-4-5-6-7-8-9/h8H,2-7H2,1H3
<b>InchiKey:</b>	NUJGJRNETVAIRJ-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O
<b>SMILES:</b>	CCCCCCCC=O
<b>Mol. weight [g/mol]:</b>	128.21
<b>CAS:</b>	124-13-0

## Physical Properties

Property code	Value	Unit	Source
chl	-5100.04	kJ/mol	NIST Webbook
gf	-83.04	kJ/mol	Joback Method
hf	-291.90 ± 2.80	kJ/mol	NIST Webbook
hfus	18.77	kJ/mol	Joback Method
hvap	51.00 ± 0.30	kJ/mol	NIST Webbook
hvap	53.80	kJ/mol	NIST Webbook
hvap	43.00 ± 0.20	kJ/mol	NIST Webbook
hvap	51.30 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.36		Aqueous Solubility Prediction Method

logp	2.546		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2740.00	kPa	KDB
pc	2960.00 ± 50.00	kPa	NIST Webbook
rhoc	262.83 ± 3.85	kg/m3	NIST Webbook
rinpol	157.60		NIST Webbook
rinpol	160.80		NIST Webbook
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sl	365.40	J/molxK	NIST Webbook
tb	444.90	K	KDB
tb	444.20	K	NIST Webbook
tb	441.65 ± 3.00	K	NIST Webbook
tb	445.15 ± 3.00	K	NIST Webbook
tb	441.65 ± 3.00	K	NIST Webbook
tc	638.10 ± 0.80	K	NIST Webbook
tc	621.10	K	KDB
tc	639.30 ± 0.30	K	NIST Webbook
tf	246.00	K	KDB
tf	247.72 ± 0.10	K	NIST Webbook
tf	260.82	K	Aqueous Solubility Prediction Method
vc	0.500	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.76	J/molxK	516.49	Joback Method
cpg	312.85	J/molxK	573.42	Joback Method
cpg	302.52	J/molxK	544.95	Joback Method
cpg	322.76	J/molxK	601.88	Joback Method
cpg	256.71	J/molxK	431.10	Joback Method
cpg	268.86	J/molxK	459.56	Joback Method
cpg	280.54	J/molxK	488.03	Joback Method
dvisc	0.0009650	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	0.0012000	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)
dvisc	0.0010740	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)
hfust	25.86	kJ/mol	288.20	NIST Webbook
hfust	25.86	kJ/mol	288.20	NIST Webbook
hvapt	43.40	kJ/mol	365.50	NIST Webbook
rhol	836.10	kg/m <sup>3</sup>	298.20	Physical Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.2 K

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.20	K	2.70	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57402e+01
Coeff. B	-4.22158e+03



Coeff. C	-6.46240e+01
Temperature range (K), min.	337.82
Temperature range (K), max.	469.43

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	2.62505e+02
Coeff. B	-1.60884e+04
Coeff. C	-3.73436e+01
Coeff. D	2.99392e-05
Temperature range (K), min.	246.00
Temperature range (K), max.	621.00

## Sources

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Thermodynamic Properties of Mixtures Containing Ionic Liquids. 9. Activity Coefficient at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes	<a href="https://www.doi.org/10.1021/je0503554">https://www.doi.org/10.1021/je0503554</a>
Joback Method for Estimation of Dynamic Viscosity of Several Aldehydes	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Joback Method for Estimation of Dynamic Viscosity of Several Aldehydes	<a href="https://www.doi.org/10.1021/je0502344">https://www.doi.org/10.1021/je0502344</a>
Joback Method for Estimation of Dynamic Viscosity of Several Aldehydes	<a href="https://www.thermo.com/files/research/kdb/mol/mol1239.mol">https://www.thermo.com/files/research/kdb/mol/mol1239.mol</a>
Joback Method for Estimation of Dynamic Viscosity of Several Aldehydes	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1239">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1239</a>
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 9. Activity Coefficient at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes	<a href="https://www.doi.org/10.1021/je050440b">https://www.doi.org/10.1021/je050440b</a>
Joback Method for Estimation of Dynamic Viscosity of Several Aldehydes	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
Joback Method for Estimation of Dynamic Viscosity of Several Aldehydes	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C124130&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C124130&amp;Units=SI</a>
Joback Method for Estimation of Dynamic Viscosity of Several Aldehydes	<a href="https://www.doi.org/10.1021/acs.jced.8b00086">https://www.doi.org/10.1021/acs.jced.8b00086</a>
Joback Method for Estimation of Dynamic Viscosity of Several Aldehydes	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
Aqueous Solubility Prediction Method: McGowan Method:	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions

<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rhoc:</b>	Critical density
<b>rhoL:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sl:</b>	Liquid phase molar entropy at standard conditions
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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