

# Hexanal

<b>Other names:</b>	1-Hexanal 1-pentanecarbaldehyde Aldehyde C-6 CAPROALDEHYDE Caproic aldehyde Capronaldehyde HEXALDEHYDE Hexan-1-al Hexanaldehyde Hexylaldehyde Kapronaldehyd N-CAPROALDEHYDE NSC 2596 UN 1207 n-C5H11CHO n-Capronaldehyde n-Caproylaldehyde n-Hexaldehyde n-Hexanal
<b>Inchi:</b>	InChI=1S/C6H12O/c1-2-3-4-5-6-7/h6H,2-5H2,1H3
<b>InchiKey:</b>	JARKCYVAAOWBJS-UHFFFAOYSA-N
<b>Formula:</b>	C6H12O
<b>SMILES:</b>	CCCCCC=O
<b>Mol. weight [g/mol]:</b>	100.16
<b>CAS:</b>	66-25-1

## Physical Properties

Property code	Value	Unit	Source
af	0.4590		KDB
gf	-99.88	kJ/mol	Joback Method
hf	-252.75	kJ/mol	Joback Method
hfus	13.58	kJ/mol	Joback Method
hvap	42.30 ± 0.10	kJ/mol	NIST Webbook
hvap	42.50 ± 0.40	kJ/mol	NIST Webbook
ie	9.72 ± 0.01	eV	NIST Webbook
ie	9.62 ± 0.02	eV	NIST Webbook
ie	9.80	eV	NIST Webbook

ie	9.72 ± 0.05	eV	NIST Webbook
log10ws	-1.30		Aqueous Solubility Prediction Method
log10ws	-1.30		Estimated Solubility Method
logp	1.766		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3460.00 ± 50.00	kPa	NIST Webbook
pc	3460.00	kPa	KDB
rhoc	265.42 ± 5.01	kg/m3	NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	777.23		NIST Webbook
rinpol	778.46		NIST Webbook
rinpol	748.40		NIST Webbook
rinpol	780.00		NIST Webbook
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ripol	1093.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1087.00	NIST Webbook
ripol	1101.00	NIST Webbook
ripol	1098.00	NIST Webbook
ripol	1077.00	NIST Webbook

ripol	1086.00	NIST Webbook
ripol	1091.00	NIST Webbook
ripol	1084.00	NIST Webbook
ripol	1084.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1101.00	NIST Webbook
ripol	1085.00	NIST Webbook
ripol	1093.00	NIST Webbook
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ripol	1093.00	NIST Webbook
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ripol	1093.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1084.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1084.00	NIST Webbook
ripol	1091.00	NIST Webbook
ripol	1083.00	NIST Webbook
ripol	1079.00	NIST Webbook
ripol	1100.00	NIST Webbook
ripol	1081.00	NIST Webbook
ripol	1051.00	NIST Webbook
ripol	1077.00	NIST Webbook
ripol	1074.00	NIST Webbook
ripol	1090.00	NIST Webbook
ripol	1075.00	NIST Webbook
ripol	1127.00	NIST Webbook
ripol	1083.00	NIST Webbook
ripol	1083.00	NIST Webbook
ripol	1075.00	NIST Webbook
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ripol	1083.00	NIST Webbook
ripol	1127.00	NIST Webbook
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ripol	1074.00	NIST Webbook
ripol	1081.00	NIST Webbook
ripol	1110.00	NIST Webbook
ripol	1062.00	NIST Webbook
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ripol	1076.00	NIST Webbook

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ripol	1078.00		NIST Webbook
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ripol	1083.00		NIST Webbook
ripol	1059.00		NIST Webbook
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ripol	1094.00		NIST Webbook
ripol	1078.00		NIST Webbook
ripol	1078.00		NIST Webbook
ripol	1073.00		NIST Webbook
ripol	1084.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1084.00		NIST Webbook
ripol	1079.00		NIST Webbook
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ripol	1099.00		NIST Webbook
ripol	1049.00		NIST Webbook
ripol	1077.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1110.00		NIST Webbook
ripol	1114.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1108.00		NIST Webbook
sl	280.30	J/molxK	NIST Webbook
tb	404.00	K	KDB
tb	401.90	K	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tc	592.80 ± 2.50	K	NIST Webbook
tc	591.00 ± 0.80	K	NIST Webbook
tc	591.00	K	KDB
tf	217.00	K	KDB
tf	216.90 ± 2.00	K	NIST Webbook
tf	211.90 ± 2.00	K	NIST Webbook
tt	214.93 ± 0.06	K	NIST Webbook
vc	0.389	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.76	J/mol×K	471.56	Joback Method
cpg	232.79	J/mol×K	557.77	Joback Method
cpg	224.79	J/mol×K	529.04	Joback Method
cpg	216.44	J/mol×K	500.30	Joback Method
cpg	179.56	J/mol×K	385.34	Joback Method
cpg	189.32	J/mol×K	414.08	Joback Method
cpg	198.72	J/mol×K	442.82	Joback Method
cpl	210.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0008050	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	0.0007160	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	0.0006390	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)
hfust	13.33	kJ/mol	214.94	NIST Webbook
hvapt	41.00	kJ/mol	358.50	NIST Webbook
hvapt	40.80	kJ/mol	362.00	NIST Webbook

pvap	99.72	kPa	402.17	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	47.56	kPa	377.98	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	5.18	kPa	322.27	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	6.00	kPa	325.43	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	6.71	kPa	327.84	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	7.51	kPa	330.22	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	8.71	kPa	333.56	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	10.99	kPa	338.89	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	12.59	kPa	342.12	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	15.55	kPa	347.22	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	19.80	kPa	353.44	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	25.45	kPa	360.11	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one



pvap	31.91	kPa	366.28	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	38.88	kPa	371.95	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
rho1	830.01	kg/m <sup>3</sup>	298.15	Liquid-liquid equilibria and density data for pseudoternary systems of refined soybean oil + (hexanal, or heptanal, or butyric acid, or valeric acid, or caproic acid, or caprylic acid) + dimethyl sulfoxide at 298.15 K
sfust	62.00	J/molxK	214.94	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	425.80	K	190.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	358.10	K	24.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	367.30	K	34.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa

tbp	374.20	K	43.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	380.00	K	53.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	385.30	K	62.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	389.90	K	72.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	394.00	K	81.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	397.80	K	91.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	404.90	K	110.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa

tbp	407.90	K	119.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	410.60	K	129.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	413.40	K	138.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	416.00	K	148.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	418.60	K	157.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	420.80	K	167.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	422.80	K	176.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa

tbp	424.90	K	186.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbrp	301.20	K	1.60	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44833e+01
Coeff. B	-3.38781e+03
Coeff. C	-5.85800e+01
Temperature range (K), min.	297.23
Temperature range (K), max.	427.95

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.73059e+01
Coeff. B	-7.96236e+03
Coeff. C	-1.06744e+01
Coeff. D	7.04921e-06
Temperature range (K), min.	217.15
Temperature range (K), max.	579.00

## Sources

### KDB Vapor Pressure Data:

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1237>

Activity Coefficients at Infinite Dilution of Volatile Compounds in Water: Effect of Temperature and Salt Concentration. Infinite dilution of organic solutes in benzene and cyclohexane. Viscosity of Several Aldehydes. Fragrance Compounds in the Air. Vapor Pressure of Organic Compounds (298.15 K, 308.15 K, and 318.15 K): Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa. Activity Coefficients for Hexanal, 2-Methylbutanal, 3-Methylbutanal, and Dimethylsulfide in Water at (98.1 to 99.0) deg C:

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<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

<https://www.doi.org/10.1016/j.jct.2014.03.006>

<https://www.doi.org/10.1021/je060324o>

Experimental Study of Thermodynamic Properties of Mixtures Containing Ionic Liquids: Cationic 1-methylimidazolium Ethyl Sulfate Using Gas-Liquid Chromatography and Transpiration for pseudoternary systems of refined soybean oil + (hexanal, or heptanal, or butyric acid, or valeric acid, or caproic acid, or caprylic acid) + dimethyl sulfoxide at 298.15 K: High-pressure (vapor + liquid) equilibria for binary systems Solubilities of Hexanal, Benzaldehyde, and p-cymene in Phenol and Ethanol: Methods and Estimated Solubility Method: Water at Temperatures between (50 and 100) deg C.

High-pressure (vapour + liquid) equilibria for ternary systems McGowan's Method: (2-hexenal or hexanal + carbon dioxide + water): Partition Coefficient measurement: Thermodynamic Properties of Mixtures Containing Ionic Liquids. 8. Activity Coefficients in Nonelectrolyte Mixtures Containing Ionic Liquids. Estimation of Equilibrium Constants and Enthalpy Changes and High-Pressure Vapor-Liquid Equilibria of Bis(trifluoromethylsulfonyl) Imide Using Gas-Liquid Chromatography and Static Method:

<https://www.doi.org/10.1021/je0602723>  
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
<https://www.doi.org/10.1016/j.jct.2018.10.030>  
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<https://www.doi.org/10.1016/j.jct.2015.05.003>  
<http://link.springer.com/article/10.1007/BF02311772>  
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C66251&Units=SI>

## Legend

af: Acentric Factor  
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  
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  
ie: Ionization energy  
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

<b>tb:</b>	Normal Boiling Point Temperature
<b>tbp:</b>	Boiling point at given pressure
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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