

Heptanal

Other names:	1-Heptaldehyde
	1-Heptanal
	1-hexanecarbaldehyde
	ENANTHAL
	ENANTHIC ALDEHYDE
	Enanthaldehyde
	Enanthole
	Heptaldehyde
	Heptan-1-al
	Heptanaldehyde
	Heptyl aldehyde
	N-HEPTALDEHYDE
	NSC 2190
	Oenanthal
	Oenanthaldehyde
	Oenanthic aldehyde
	Oenanthol
	n-C6H13CHO
	n-Heptanal
	n-Heptylaldehyde
Inchi:	InChI=1S/C7H14O/c1-2-3-4-5-6-7-8/h7H,2-6H2,1H3
InchiKey:	FXHGMKSSBGDXIY-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CCCCCCC=O
Mol. weight [g/mol]:	114.19
CAS:	111-71-7

Physical Properties

Property code	Value	Unit	Source
af	0.2590		KDB
chl	-4444.00 ± 4.00	kJ/mol	NIST Webbook
gf	-91.46	kJ/mol	Joback Method
hf	-264.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-312.00 ± 4.00	kJ/mol	NIST Webbook
hfus	16.18	kJ/mol	Joback Method
hvap	47.30 ± 0.10	kJ/mol	NIST Webbook
hvap	48.00 ± 1.00	kJ/mol	NIST Webbook

hvap	48.00	kJ/mol	NIST Webbook
hvap	48.00 ± 1.30	kJ/mol	NIST Webbook
hvap	48.70	kJ/mol	NIST Webbook
ie	9.65 ± 0.02	eV	NIST Webbook
log10ws	-1.70		Aqueous Solubility Prediction Method
logp	2.156		Crippen Method
mcpvol	111.060	ml/mol	McGowan Method
pc	3160.00 ± 25.00	kPa	NIST Webbook
pc	3030.00	kPa	KDB
rhoc	262.63 ± 4.57	kg/m3	NIST Webbook
rinpol	860.00		NIST Webbook
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ripol	1184.00	NIST Webbook
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ripol	1186.00	NIST Webbook
ripol	1196.00	NIST Webbook
ripol	1186.00	NIST Webbook
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ripol	1181.00	NIST Webbook
ripol	1180.00	NIST Webbook
ripol	1181.00	NIST Webbook
ripol	1174.00	NIST Webbook
ripol	1190.00	NIST Webbook
ripol	1190.00	NIST Webbook

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ripol	1184.00		NIST Webbook
ripol	1189.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1189.00		NIST Webbook
ripol	1195.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1182.00		NIST Webbook
sg	461.50 ± 4.20	J/mol×K	NIST Webbook
sl	335.40	J/mol×K	NIST Webbook
sl	348.50	J/mol×K	NIST Webbook
tb	425.00	K	KDB
tc	616.70 ± 0.60	K	NIST Webbook
tc	161.80 ± 0.40	K	NIST Webbook
tc	638.50	K	KDB
tf	230.07	K	Aqueous Solubility Prediction Method
tf	230.00	K	KDB
tt	229.20 ± 0.02	K	NIST Webbook
tt	229.80 ± 0.20	K	NIST Webbook
vc	0.445	m3/kmol	KDB
zc	0.2536980		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.56	J/mol×K	522.69	Joback Method
cpg	267.94	J/mol×K	551.31	Joback Method
cpg	216.98	J/mol×K	408.22	Joback Method
cpg	228.00	J/mol×K	436.84	Joback Method
cpg	238.59	J/mol×K	465.46	Joback Method
cpg	248.78	J/mol×K	494.08	Joback Method
cpg	276.95	J/mol×K	579.93	Joback Method
cpl	250.33	J/mol×K	298.15	NIST Webbook
cpl	204.60	J/mol×K	298.00	NIST Webbook
cpl	230.78	J/mol×K	298.15	NIST Webbook
dvisc	0.0004120	Pa×s	375.29	Joback Method
dvisc	0.0003210	Pa×s	408.22	Joback Method
dvisc	0.0046356	Pa×s	210.65	Joback Method
dvisc	0.0021988	Pa×s	243.58	Joback Method
dvisc	0.0012457	Pa×s	276.51	Joback Method

dvisc	0.0007965	Pa×s	309.43	Joback Method
dvisc	0.0005550	Pa×s	342.36	Joback Method
hfust	22.89	kJ/mol	229.30	NIST Webbook
hfust	23.59	kJ/mol	229.80	NIST Webbook
hfust	22.89	kJ/mol	229.30	NIST Webbook
hvapt	62.00	kJ/mol	356.50	NIST Webbook
hvapt	47.75	kJ/mol	425.00	KDB
rho1	816.83	kg/m3	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	102.63	J/mol×K	229.80	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.80	K	4.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56266e+01
Coeff. B	-4.04483e+03
Coeff. C	-5.95640e+01
Temperature range (K), min.	323.26
Temperature range (K), max.	451.69

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.14364e+02
Coeff. B	-9.97308e+03
Coeff. C	-1.44580e+01
Coeff. D	7.06940e-06
Temperature range (K), min.	230.15
Temperature range (K), max.	603.00

Sources

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Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McCowan Method:	http://link.springer.com/article/10.1007/BF02311772
1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl) Imide	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 9. Activity Coefficients at Infinite Dilution for pseudoternary systems of refined aromatic hydrocarbons, alcohols, esters, and aldehydes in:	https://www.doi.org/10.1021/je050440b
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 9. Activity Coefficients at Infinite Dilution for pseudoternary systems of refined aromatic hydrocarbons, alcohols, esters, and aldehydes in:	https://www.doi.org/10.1016/j.jct.2018.10.030
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Thermodynamic Properties of Mixtures Containing Ionic Liquids. 9. Activity Coefficients at Infinite Dilution for pseudoternary systems of refined aromatic hydrocarbons, alcohols, esters, and aldehydes in:	https://www.thermo.com/files/research/kdb/mol/mol1238.mol
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1238
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
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
hfl:	Liquid phase 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
rhof:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
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
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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