Octanoic acid

Other names:	1-Heptanecarboxylic acid
	1-Octanoic acid
	C-8 Acid
	Caprylic acid
	Emery 657
	Enantic acid
	Heptane-1-carboxylic acid
	Hexacid 898
	Kyselina kaprylova
	Lunac 8-95
	NSC 5024
	Neo-Fat 8
	Octic acid
	Octoic acid
	Octylic acid
	Prifac 2901
	Prifrac 2901
	n-Caprylic acid
	n-Octanoic acid
	n-Octoic acid
	n-Octylic acid
Inchi:	InChI=1S/C8H16O2/c1-2-3-4-5-6-7-8(9)10/h2-7H2,1H3,(H,9,10)
InchiKey:	WWZKQHOCKIZLMA-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCCCCC(=O)O
Mol. weight [g/mol]:	144.21
CAS:	124-07-2

Physical Properties

Property code	Value	Unit	Source
chl	-4797.92 ± 0.54	kJ/mol	NIST Webbook
chl	-4799.90 ± 0.80	kJ/mol	NIST Webbook
gf	-249.26	kJ/mol	Joback Method
hf	-556.60 ± 1.10	kJ/mol	NIST Webbook
hf	-554.00 ± 1.10	kJ/mol	NIST Webbook
hf	-556.60	kJ/mol	NIST Webbook

hf	-554.50 ± 1.30	kJ/mol	NIST Webbook
hfl	-634.80 ± 0.80	kJ/mol	NIST Webbook
hfl	-636.89 ± 0.54	kJ/mol	NIST Webbook
hfus	22.16	kJ/mol	Joback Method
hsub	113.00 ± 6.00	kJ/mol	NIST Webbook
hvap	81.00 ± 0.60	kJ/mol	NIST Webbook
hvap	81.20	kJ/mol	NIST Webbook
hvap	82.90 ± 1.00	kJ/mol	NIST Webbook
hvap	82.90 ± 1.00	kJ/mol	NIST Webbook
hvap	80.30	kJ/mol	NIST Webbook
log10ws	-2.30		Aqueous Solubility Prediction Method
logp	2.432		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2640.00	kPa	KDB
pc	2869.00 ± 60.00	kPa	NIST Webbook
pc	2700.00 ± 250.00	kPa	NIST Webbook
pc	2565.44 ± 90.00	kPa	NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1166.00		NIST Webbook
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tc	695.00	K	KDB
tf	289.63	K	The solid liquid phase diagrams of binary mixtures of even saturated fatty acids differing by six carbon atoms
tf	289.86	K	High pressure solid liquid equilibria of fatty acids
tf	289.40	K	KDB
tf	289.61	K	Aqueous Solubility Prediction Method
tt	289.66 ± 0.02	K	NIST Webbook
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.45	J/mol×K	528.49	Joback Method
cpg	368.11	J/mol×K	697.39	Joback Method
cpg	359.37	J/mol×K	669.24	Joback Method
cpg	350.23	J/mol×K	641.09	Joback Method
cpg	340.68	J/mol×K	612.94	Joback Method

cpg	330.71	J/mol×K	584.79	Joback Method
cpg	320.30	J/mol×K	556.64	Joback Method
cpl	297.92	J/mol×K	298.15	NIST Webbook
cpl	304.60	J/mol×K	305.00	NIST Webbook
dvisc	0.0161114	Pa×s	290.67	Joback Method
dvisc	0.0046128	Pa×s	330.31	Joback Method
dvisc	0.0017266	Pa×s	369.94	Joback Method
dvisc	0.0007817	Pa×s	409.58	Joback Method
dvisc	0.0004070	Pa×s	449.22	Joback Method
dvisc	0.0002356	Pa×s	488.85	Joback Method
dvisc	0.0001480	Pa×s	528.49	Joback Method
hfust	21.38	kJ/mol	289.70	NIST Webbook
hfust	21.38	kJ/mol	289.50	NIST Webbook
hvapt	80.00	kJ/mol	290.00	NIST Webbook
hvapt	74.40	kJ/mol	436.00	NIST Webbook
hvapt	85.30	kJ/mol	313.50	NIST Webbook
hvapt	66.60	kJ/mol	465.50	NIST Webbook
hvapt	79.80 ± 0.60	kJ/mol	320.00	NIST Webbook
hvapt	70.00	kJ/mol	407.00	NIST Webbook
rhol	910.00	kg/m3	298.15	Physico-Chemical Properties of Non-Newtonian Shear Thickening Diisopropyl-ethylammonium-Based Protic Ionic Liquids and Their Mixtures with Water and Acetonitrile
rhol	906.02	kg/m3	298.15	Excess molar enthalpies of binary systems containing 2-octanone, hexanoic acid, or octanoic acid at T = 298.15 K
rhol	906.00	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

rhol	910.30	kg/m3	290.30	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	898.20	kg/m3	308.00	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	885.90	kg/m3	323.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	873.80	kg/m3	338.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	861.80	kg/m3	353.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	849.70	kg/m3	367.80	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	837.20	kg/m3	383.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	824.60	kg/m3	398.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	812.30	kg/m3	412.90	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K

rhol	799.20	kg/m3	427.70	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
sfust	73.90	J/mol×K	289.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	417.19	K	3.47	Improving a variation of the DSC technique for measuring the boiling points of pure compounds at low pressures

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55313e+01
Coeff. B	-4.35069e+03
Coeff. C	-1.11329e+02
Temperature range (K), min.	396.74
Temperature range (K), max.	537.04

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.33561e+02
Coeff. B	-1.92069e+04
Coeff. C	-3.12560e+01
Coeff. D	1.35849e-05
Temperature range (K), min.	289.65
Temperature range (K), max.	692.00

Sources

Solubility of Small-Chain Carboxylic Acids in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je100504h
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Legend

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
hsub:	Enthalpy of sublimation at standard conditions
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume