n-Decanoic acid

Other names:	1-Decanoic acid
	1-Nonanecarboxylic acid
	Capric acid
	Caprinic acid
	Caprynic acid
	Decanoic acid
	Decanoic acid (capric acid)
	Decoic acid
	Decylic acid
	Emery 659
	Hexacid 1095
	NSC 5025
	Nonane-1-carboxylic acid
	Prifrac 296
	n-Capric acid
	n-Decoic acid
	n-Decylic acid
	neo-Fat 10
Inchi:	InChI=1S/C10H20O2/c1-2-3-4-5-6-7-8-9-10(11)12/h2-9H2,1H3,(H,11,12)
InchiKey:	GHVNFZFCNZKVNT-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCCCCCC(=O)O
Mol. weight [g/mol]:	172.26
CAS:	334-48-5

Physical Properties

Property code	Value	Unit	Source
chl	-6079.30 ± 0.90	kJ/mol	NIST Webbook
gf	-232.42	kJ/mol	Joback Method
hf	-624.20 ± 5.10	kJ/mol	NIST Webbook
hfus	28.00	kJ/mol	Solid-Liquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry
hsub	119.00 ± 2.00	kJ/mol	NIST Webbook
hsub	130.00 ± 5.00	kJ/mol	NIST Webbook

hsub	118.80 ± 2.20	kJ/mol	NIST Webbook
hvap	61.28	kJ/mol	Joback Method
log10ws	-3.44		Aqueous Solubility Prediction Method
logp	3.212		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2230.00	kPa	KDB
pc	2161.74 ± 90.00	kPa	NIST Webbook
pc	2100.00 ± 400.00	kPa	NIST Webbook
pt	9.73e-05 ± 2.67e-05	kPa	NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	234.82		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1380.00		NIST Webbook
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ripol	2278.00		NIST Webbook
ripol	2300.00		NIST Webbook
tb	535.65 ± 5.00	K	NIST Webbook
tb	541.65 ± 3.00	K	NIST Webbook
tb	541.90	K	KDB
tb	543.20	K	NIST Webbook
tb	541.00 ± 2.00	K	NIST Webbook
tb	542.15 ± 3.00	K	NIST Webbook
tb	541.95 ± 1.00	K	NIST Webbook

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tb	544.15 ± 3.00	K	NIST Webbook
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tc	720.53 ± 3.00	K	NIST Webbook
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tf	303.40 ± 0.50	K	NIST Webbook
tf	305.00 ± 3.00	K	NIST Webbook
tf	302.90 ± 1.50	K	NIST Webbook
tf	304.00 ± 1.60	K	NIST Webbook
tf	304.70 ± 0.05	K	NIST Webbook
tf	304.42	K	Solid-Liquid Equilibrium of Binary Fatty Acid Mixtures
tf	305.15	K	Prediction of the properties of eutectic fatty acid phase change materials
tf	305.46	K	The solid liquid phase diagrams of binary mixtures of even saturated fatty acids differing by six carbon atoms
tf	305.22	K	Solid-liquid phase equilibrium diagrams of binary mixtures containing fatty acids, fatty alcohol compounds and tripalmitin using differential scanning calorimetry
tf	304.75	K	Measurement and PC-SAFT modeling of solid-liquid equilibrium of deep eutectic solvents of quaternary ammonium chlorides and carboxylic acids
tf	305.14	K	KDB
tf	304.53	K	Aqueous Solubility Prediction Method
tf	304.40 ± 0.20	K	NIST Webbook
tf	304.15 ± 2.00	K	NIST Webbook
tf	300.10 ± 1.00	K	NIST Webbook
tf	304.60 ± 2.00	K	NIST Webbook
tf	303.90 ± 1.00	K	NIST Webbook
tt	304.55 ± 0.02	K	NIST Webbook
tt	303.95 ± 0.50	K	NIST Webbook
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.86	J/mol×K	741.22	Joback Method
cpg	415.22	J/mol×K	602.08	Joback Method
cpg	402.78	J/mol×K	574.25	Joback Method
cpg	449.45	J/mol×K	685.56	Joback Method
cpg	459.89	J/mol×K	713.39	Joback Method
cpg	438.54	J/mol×K	657.73	Joback Method
cpg	427.13	J/mol×K	629.91	Joback Method
cps	475.59	J/mol×K	298.15	NIST Webbook
cps	361.10	J/mol×K	285.00	NIST Webbook
dvisc	0.0001652	Pa×s	530.74	Joback Method
dvisc	0.0002839	Pa×s	487.24	Joback Method
dvisc	0.0005426	Pa×s	443.73	Joback Method
dvisc	0.0011935	Pa×s	400.22	Joback Method
dvisc	0.0001044	Pa×s	574.25	Joback Method
dvisc	0.0111394	Pa×s	313.21	Joback Method
dvisc	0.0031819	Pa×s	356.72	Joback Method
hfust	27.99	kJ/mol	304.50	NIST Webbook
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hsubt	117.00 ± 2.00	kJ/mol	289.80	NIST Webbook
hsubt	117.10 ± 1.70	kJ/mol	295.50	NIST Webbook
hvapt	76.40	kJ/mol	470.50	NIST Webbook
hvapt	88.60	kJ/mol	314.00	NIST Webbook
hvapt	71.40	kJ/mol	418.00	NIST Webbook
rhol	784.90	kg/m3	442.20	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	772.90	kg/m3	457.20	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K

rhol	761.90	kg/m3	472.20	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	796.40	kg/m3	428.20	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	797.20	kg/m3	427.20	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	812.20	kg/m3	408.20	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	827.30	kg/m3	388.30	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	843.10	kg/m3	368.30	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	855.30	kg/m3	352.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	878.00	kg/m3	322.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	871.00	kg/m3	332.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K

sfust	97.40	J/mol×K	300.10	NIST Webbook
sfust	92.00	J/mol×K	304.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.20	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62028e+01
Coeff. B	-4.40263e+03
Coeff. C	-1.49953e+02
Temperature range (K), min.	426.58
Temperature range (K), max.	554.19

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.88007e+02
Coeff. B	-3.39121e+04
Coeff. C	-6.83540e+01
Coeff. D	3.21849e-05
Temperature range (K), min.	304.75
Temperature range (K), max.	713.00

Sources

Physical properties of systems of interest to the edible oil industry: Viscosities and densities of model systems formed by (triacylglycerol + fatty acid + solvent)	https://www.doi.org/10.1016/j.jct.2017.06.012
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Measurement and PC-SAFT modeling of solid-liquid equilibrium of deep eutectic solvents of quaternary ammonium chlorides and carboxylic acids:	https://www.doi.org/10.1016/j.fluid.2017.04.007

Thermodynamic properties of hydrophobic deep eutectic solvents and solubility of water and HMF in them:	https://www.doi.org/10.1016/j.fluid.2019.02.010
The solid-liquid phase diagrams of binary mixtures of even saturated fatty acids containing by six carbon atoms:	https://www.doi.org/10.1016/j.tca.2009.06.018
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Solid-Liquid Equilibrium of Binary Fatty Acid Mixtures:	https://www.doi.org/10.1021/je060146z
Viscosities of Fatty Mixtures: Experimental Data and Prediction:	https://www.doi.org/10.1021/je700293s
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=944
Solid-Liquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry:	https://www.doi.org/10.1021/acs.jced.8b01006
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C334485&Units=SI
Carbon Dioxide Solubilities in Decanoic Acid-Based Hydrophobic Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.7b00534
Prediction of the properties of eutectic fatty acid phase change materials:	https://www.doi.org/10.1016/j.tca.2017.12.024
Phase Equilibria of Long-Chain Carboxylic Acids in Supercritical Propane:	https://www.doi.org/10.1021/je101077v
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid 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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
pt:	Triple Point 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume