

Heptanoic acid

Other names:	1-Heptanoic acid
	1-Hexanecarboxylic acid
	Enanthic acid
	Enanthylic acid
	Hepthlic acid
	Heptoic acid
	Heptylic acid
	Hexacid C-7
	N-OENANTHIC ACID
	NSC 2192
	Oenanthic acid
	Oenanthylic acid
	n-Heptanoic acid
	n-Heptoic acid
	n-Heptylic acid
Inchi:	InChI=1S/C7H14O2/c1-2-3-4-5-6-7(8)9/h2-6H2,1H3,(H,8,9)
InchiKey:	MNWFXJYAOYHMED-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCCCCCC(=O)O
Mol. weight [g/mol]:	130.18
CAS:	111-14-8

Physical Properties

Property code	Value	Unit	Source
chl	-4146.90 ± 0.90	kJ/mol	NIST Webbook
chl	-4144.00 ± 0.59	kJ/mol	NIST Webbook
gf	-257.68	kJ/mol	Joback Method
hf	-536.50 ± 1.70	kJ/mol	NIST Webbook
hf	-539.50 ± 1.60	kJ/mol	NIST Webbook
hf	-539.50 ± 1.60	kJ/mol	NIST Webbook
hfl	-608.50 ± 0.90	kJ/mol	NIST Webbook
hfl	-611.49 ± 0.59	kJ/mol	NIST Webbook
hfus	19.57	kJ/mol	Joback Method
hvap	72.00 ± 1.50	kJ/mol	NIST Webbook
hvap	72.90 ± 0.80	kJ/mol	NIST Webbook
hvap	75.70	kJ/mol	NIST Webbook
hvap	72.00 ± 1.50	kJ/mol	NIST Webbook

log10ws	-1.85		Crippen Method
logp	2.041		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3161.00 ± 80.00	kPa	NIST Webbook
pc	2880.00 ± 100.00	kPa	NIST Webbook
pc	2829.63 ± 90.00	kPa	NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	176.75		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	177.80		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	176.75		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1083.00		NIST Webbook

rinpol	1080.00	NIST Webbook
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rinpol	1068.00	NIST Webbook
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rinpol	1083.00	NIST Webbook
rinpol	1069.00	NIST Webbook
ripol	1965.00	NIST Webbook
ripol	1900.00	NIST Webbook
ripol	1941.00	NIST Webbook
ripol	1950.00	NIST Webbook
ripol	1935.00	NIST Webbook
ripol	1900.00	NIST Webbook
ripol	1923.00	NIST Webbook
ripol	1933.00	NIST Webbook
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ripol	1925.00	NIST Webbook
ripol	1950.00	NIST Webbook
ripol	1956.00	NIST Webbook
ripol	1936.00	NIST Webbook
ripol	1966.00	NIST Webbook
ripol	1904.00	NIST Webbook
ripol	1975.00	NIST Webbook
ripol	1963.00	NIST Webbook
ripol	1990.00	NIST Webbook
ripol	1952.00	NIST Webbook
ripol	1950.00	NIST Webbook
ripol	1955.00	NIST Webbook
ripol	1962.00	NIST Webbook
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ripol	1977.00	NIST Webbook
ripol	1925.00	NIST Webbook
ripol	1942.00	NIST Webbook
ripol	1963.00	NIST Webbook
ripol	1916.00	NIST Webbook
ripol	1935.00	NIST Webbook
ripol	1960.00	NIST Webbook

ripol	1918.00	NIST Webbook
ripol	1965.00	NIST Webbook
ripol	1950.00	NIST Webbook
ripol	1952.00	NIST Webbook
ripol	1928.00	NIST Webbook
ripol	1942.00	NIST Webbook
ripol	1946.00	NIST Webbook
ripol	1927.00	NIST Webbook
ripol	1932.00	NIST Webbook
ripol	1955.00	NIST Webbook
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ripol	1958.00	NIST Webbook
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ripol	2000.00	NIST Webbook
ripol	1962.00	NIST Webbook
ripol	1972.00	NIST Webbook
ripol	1976.00	NIST Webbook
ripol	1955.00	NIST Webbook
ripol	1968.00	NIST Webbook
ripol	1970.00	NIST Webbook
ripol	1934.00	NIST Webbook
ripol	1949.00	NIST Webbook
ripol	1927.00	NIST Webbook
ripol	1988.00	NIST Webbook
ripol	1986.00	NIST Webbook
ripol	1962.00	NIST Webbook
ripol	1962.00	NIST Webbook
ripol	1932.00	NIST Webbook
ripol	1924.00	NIST Webbook
ripol	1927.00	NIST Webbook
ripol	1934.00	NIST Webbook
ripol	1915.00	NIST Webbook
ripol	1958.00	NIST Webbook
ripol	1936.00	NIST Webbook
ripol	1946.00	NIST Webbook
ripol	1939.00	NIST Webbook
ripol	1916.00	NIST Webbook

ripol	1950.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1953.00		NIST Webbook
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ripol	1965.00		NIST Webbook
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ripol	1918.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1976.00		NIST Webbook
ripol	1971.00		NIST Webbook
sl	323.35	J/mol×K	NIST Webbook
tb	505.61	K	Joback Method
tc	677.80 ± 2.00	K	NIST Webbook
tc	679.00 ± 1.00	K	NIST Webbook
tc	683.52 ± 3.00	K	NIST Webbook
tf	264.00 ± 2.00	K	NIST Webbook
tf	265.69 ± 0.30	K	NIST Webbook
tf	266.00 ± 2.00	K	NIST Webbook
tf	263.00 ± 2.00	K	NIST Webbook
tf	266.00 ± 0.05	K	NIST Webbook
tt	265.83 ± 0.02	K	NIST Webbook
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.53	J/mol×K	505.61	Joback Method
cpg	319.29	J/mol×K	675.71	Joback Method
cpg	302.90	J/mol×K	619.01	Joback Method

cpg	294.15	J/mol×K	590.66	Joback Method
cpg	285.01	J/mol×K	562.31	Joback Method
cpg	275.47	J/mol×K	533.96	Joback Method
cpg	311.28	J/mol×K	647.36	Joback Method
cpl	267.31	J/mol×K	298.15	NIST Webbook
cpl	265.43	J/mol×K	298.15	NIST Webbook
dvisc	0.0055318	Pa×s	317.10	Joback Method
dvisc	0.0001754	Pa×s	505.61	Joback Method
dvisc	0.0002800	Pa×s	467.91	Joback Method
dvisc	0.0004852	Pa×s	430.21	Joback Method
dvisc	0.0020686	Pa×s	354.80	Joback Method
dvisc	0.0192902	Pa×s	279.40	Joback Method
dvisc	0.0009345	Pa×s	392.50	Joback Method
hfust	15.44	kJ/mol	265.80	NIST Webbook
hvapt	76.00	kJ/mol	266.00	NIST Webbook
hvapt	72.50 ± 0.80	kJ/mol	305.50	NIST Webbook
hvapt	69.00	kJ/mol	433.00	NIST Webbook
hvapt	68.30	kJ/mol	423.00	NIST Webbook
pvap	24.65	kPa	451.00	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	20.63	kPa	446.40	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	16.57	kPa	441.33	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid

pvap	12.56	kPa	435.07	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	8.63	kPa	426.48	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	4.70	kPa	413.48	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	27.67	kPa	453.80	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
rfi	1.41750		295.10	Ternary Liquid-Liquid Equilibria of Acetonitrile and Water with Heptanoic Acid and Nonanol at 323.15 K and 1 atm
rfi	1.41720		293.15	Vapour-liquid equilibrium of propionic acid + caproic acid, isobutyric acid + caproic acid, valeric acid + caproic acid and caproic acid + enanthoic acid binary mixtures

rhoI	909.29	kg/m3	303.15	Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures
rhoI	920.60	kg/m3	290.30	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	905.70	kg/m3	308.00	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	893.00	kg/m3	323.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	880.40	kg/m3	338.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	867.80	kg/m3	353.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	855.40	kg/m3	367.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	842.30	kg/m3	383.20	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K

rhoI	829.40	kg/m3	397.90	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	816.60	kg/m3	412.90	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	803.40	kg/m3	427.70	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	918.00	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
rhoI	913.47	kg/m3	298.15	Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures
rhoI	917.65	kg/m3	293.15	Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures
rhoI	905.10	kg/m3	308.15	Effect of temperature on density, sound velocity, refractive index and their derived properties for the binary systems (heptanoic acid + propanoic or butanoic acids)

rhoI	909.30	kg/m3	303.15	Effect of temperature on density, sound velocity, refractive index and their derived properties for the binary systems (heptanoic acid + propanoic or butanoic acids)
rhoI	913.50	kg/m3	298.15	Effect of temperature on density, sound velocity, refractive index and their derived properties for the binary systems (heptanoic acid + propanoic or butanoic acids)
rhoI	917.70	kg/m3	293.15	Effect of temperature on density, sound velocity, refractive index and their derived properties for the binary systems (heptanoic acid + propanoic or butanoic acids)
rhoI	900.94	kg/m3	313.15	Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures
rhoI	905.11	kg/m3	308.15	Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures
rhoI	900.90	kg/m3	313.15	Effect of temperature on density, sound velocity, refractive index and their derived properties for the binary systems (heptanoic acid + propanoic or butanoic acids)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.20	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49666e+01
Coeff. B	-3.84187e+03
Coeff. C	-1.23742e+02
Temperature range (K), min.	385.47
Temperature range (K), max.	521.65

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	3.31594e+02
Coeff. B	-2.35518e+04
Coeff. C	-4.59654e+01
Coeff. D	2.35250e-05
Temperature range (K), min.	265.83
Temperature range (K), max.	680.00

Sources

Physico-Chemical Properties of Non-Newtonian Shear Thickening Dispersions and Other Based on the Viscosity of the Dispersions of Eight Carboxylic Acids with Water and Acetonitrile. <https://www.doi.org/10.1021/je101191e>

Conductivity of Electrolyte Mixtures with Water and Acetonitrile. <https://www.doi.org/10.1021/acs.jced.5b00971>

Thermodynamic Properties of the binary systems (heptanoic acid + propanoic or butanoic acids). <https://www.doi.org/10.1016/j.jct.2014.06.004>

General Method for the binary systems (heptanoic acid + propanoic or butanoic acids). https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: https://en.wikipedia.org/wiki/Joback_method

Ternary Liquid-Liquid Equilibria of Acetonitrile and Water with Heptanoic Acid and Nonanol at 323.15 K and 1 atm: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C111148&Units=SI>

<https://www.doi.org/10.1021/je800404f>

Vapour-liquid equilibrium of propionic acid + caproic acid, isobutyric acid + caproic acid, and isobutyric acid + propionic acid
Temperature and thermophysical acid properties of small chain acids and their blends in supercritical Carbon Dioxide:
Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/cj990307l>

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<https://www.chemeo.com/cid/32-217-5/Heptanoic-acid.pdf>

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