

Hexanoic acid, ethyl ester

Other names:	8068-81-3 Acetic acid, butyl-, ethyl ester Caproic acid ethyl ester Ethyl butyl acetate Ethyl caproate Ethyl ester of hexanoic acid Ethyl hexanoate Ethyl hexoate Ethyl n-hexanoate NSC 8882 n-Caproic acid ethyl ester
Inchi:	InChI=1S/C8H16O2/c1-3-5-6-7-8(9)10-4-2/h3-7H2,1-2H3
InchiKey:	SHZIWNPUGXLXDT-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCCC(=O)OCC
Mol. weight [g/mol]:	144.21
CAS:	123-66-0

Physical Properties

Property code	Value	Unit	Source
gf	-217.44	kJ/mol	Joback Method
hf	-528.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-579.10 ± 1.10	kJ/mol	NIST Webbook
hfus	19.26	kJ/mol	Joback Method
hvap	52.00 ± 1.00	kJ/mol	NIST Webbook
hvap	50.60 ± 0.40	kJ/mol	NIST Webbook
hvap	51.72 ± 0.10	kJ/mol	NIST Webbook
hvap	51.50 ± 1.30	kJ/mol	NIST Webbook
hvap	51.10	kJ/mol	NIST Webbook
log10ws	-2.35		Estimated Solubility Method
logp	2.130		Crippen Method
mcpol	131.020	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	346.77	J/mol×K	633.80	Joback Method
cpg	336.64	J/mol×K	604.62	Joback Method
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cpg	291.94	J/mol×K	487.91	Joback Method
dvisc	0.0004290	Paxs	343.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008140	Paxs	308.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K

dvisc	0.0007570	Paxs	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007110	Paxs	318.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0007040	Paxs	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006560	Paxs	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006140	Paxs	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005760	Paxs	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005410	Paxs	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005090	Paxs	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0004820	Paxs	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0004560	Paxs	338.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0009400	Paxs	298.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0011020	Paxs	288.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0006140	Paxs	313.15	Density and Viscosity of Binary Mixtures of Ethyl-2-methylbutyrate and Ethyl Hexanoate with Methanol, Ethanol, and 1-Propanol at (293.15, 303.15, and 313.15) K

dvisc	0.0007040	Paxs	303.15	Density and Viscosity of Binary Mixtures of Ethyl-2-methylbutyrate and Ethyl Hexanoate with Methanol, Ethanol, and 1-Propanol at (293.15, 303.15, and 313.15) K
dvisc	0.0008160	Paxs	293.15	Density and Viscosity of Binary Mixtures of Ethyl-2-methylbutyrate and Ethyl Hexanoate with Methanol, Ethanol, and 1-Propanol at (293.15, 303.15, and 313.15) K
dvisc	0.0008160	Paxs	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
hvapt	50.80 ± 0.40	kJ/mol	294.00	NIST Webbook
hvapt	48.60	kJ/mol	338.00	NIST Webbook
hvapt	51.80	kJ/mol	422.50	NIST Webbook
hvapt	47.40 ± 0.30	kJ/mol	359.50	NIST Webbook
pvap	46.18	kPa	413.15	Isothermal Vapor Liquid Equilibria of n-Tetradecane + Ethyl Hexanoate, Ethyl Decanoate, and Ethyl Tetradecanoate
pvap	0.29	kPa	303.03	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	108.02	kPa	443.15	Isothermal Vapor Liquid Equilibria of n-Tetradecane + Ethyl Hexanoate, Ethyl Decanoate, and Ethyl Tetradecanoate

pvap	82.69	kPa	433.15	Isothermal Vapor Liquid Equilibria of n-Tetradecane + Ethyl Hexanoate, Ethyl Decanoate, and Ethyl Tetradecanoate
pvap	3.44e-03	kPa	253.41	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	0.01	kPa	263.26	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	0.07	kPa	283.06	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	0.14	kPa	293.05	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	16.07	kPa	382.15	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	0.56	kPa	313.15	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	1.02	kPa	323.18	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel

pvap	1.78	kPa	333.11	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	2.98	kPa	343.09	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	4.55	kPa	351.97	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	7.18	kPa	362.10	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	10.93	kPa	372.13	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	62.32	kPa	423.15	Isothermal Vapor Liquid Equilibria of n-Tetradecane + Ethyl Hexanoate, Ethyl Decanoate, and Ethyl Tetradecanoate
pvap	23.19	kPa	392.23	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	32.56	kPa	402.19	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel

pvap	44.90	kPa	412.21	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	60.62	kPa	422.19	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	80.76	kPa	432.28	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	105.57	kPa	442.29	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	136.73	kPa	452.34	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	174.60	kPa	462.43	Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel
pvap	11.35	kPa	373.15	Isothermal Vapor Liquid Equilibria of n-Tetradecane + Ethyl Hexanoate, Ethyl Decanoate, and Ethyl Tetradecanoate
pvap	16.69	kPa	383.15	Isothermal Vapor Liquid Equilibria of n-Tetradecane + Ethyl Hexanoate, Ethyl Decanoate, and Ethyl Tetradecanoate

pvap	23.94	kPa	393.15	Isothermal Vapor Liquid Equilibria of n-Tetradecane + Ethyl Hexanoate, Ethyl Decanoate, and Ethyl Tetradecanoate
pvap	33.59	kPa	403.15	Isothermal Vapor Liquid Equilibria of n-Tetradecane + Ethyl Hexanoate, Ethyl Decanoate, and Ethyl Tetradecanoate
pvap	139.11	kPa	453.15	Isothermal Vapor Liquid Equilibria of n-Tetradecane + Ethyl Hexanoate, Ethyl Decanoate, and Ethyl Tetradecanoate
rfi	1.39829		313.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40063		308.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40295		303.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.37983		353.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39360		323.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.38897		333.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.38667		338.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.38438		343.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.38210		348.15	Thermophysical properties of fatty acid methyl and ethyl esters

rfi	1.40525		298.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.37754		358.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40753		293.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40982		288.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.41210		283.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.41438		278.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39594		318.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39128		328.15	Thermophysical properties of fatty acid methyl and ethyl esters
rhoI	866.29	kg/m ³	298.15	Refractive Indices and Surface Tensions of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K
rhoI	865.59	kg/m ³	298.15	Ebulliometric Determination and Prediction of Vapor Liquid Equilibria for Binary Mixtures of Ethanol and Ethyl Hexanoate

speedsl	697.60	m/s	443.55	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	1152.70	m/s	313.34	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	1077.60	m/s	333.16	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	1046.10	m/s	343.20	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	1010.00	m/s	353.08	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa

speedsl	975.00	m/s	363.12	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	942.00	m/s	373.14	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	905.40	m/s	383.76	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	870.10	m/s	393.30	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	834.90	m/s	402.64	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa

speedsl	800.80	m/s	413.59	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	764.00	m/s	423.96	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	730.30	m/s	433.99	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	592.40	m/s	473.82	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	1191.00	m/s	301.55	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa

speedsl	1220.10	m/s	294.37	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	628.80	m/s	463.10	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	661.00	m/s	452.90	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
speedsl	1115.10	m/s	324.26	Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from (293.15 to 473.15) K and pressures from (0.1 to 10) MPa
srf	0.02	N/m	308.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	348.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

srf	0.02	N/m	338.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	328.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	318.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	298.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	288.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	358.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
tcondl	0.13	W/m×K	323.67	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase

tcondl	0.13	W/m×K	333.63	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	343.56	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	313.76	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	353.55	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	363.41	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	303.70	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	293.74	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	373.40	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	283.95	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	274.02	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase

tcondl	0.14	W/m×K	264.08	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.15	W/m×K	254.29	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	383.37	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48813e+01
Coeff. B	-3.87622e+03
Coeff. C	-6.35120e+01
Temperature range (K), min.	329.12
Temperature range (K), max.	468.56

Sources

NIST Webbook:

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Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Decanoate, and Ethyl Dodecanoate in the Temperature Range 293.15 to 318.15 K: Prediction of Vapor-Liquid Equilibria by the UNIFAC Method. *Journal of Chemical Engineering Data*, 2015, 60 (1), 1-15. DOI: 10.1021/acs.jced.5b00115

Speed of sound measurement and prediction of ethyl hexanoate and ethyl octanoate at temperatures from 293.15 to 318.15 K. *Journal of Chemical Engineering Data*, 2018, 63 (7), 2531-2535. DOI: 10.1021/acs.jced.8b00115

Solubilities of CO₂ capture absorbents methyl formate, ethyl hexanoate and methyl formate plus hexanoate in the liquid phase. *Journal of Chemical Engineering Data*, 2019, 64 (1), 1-15. DOI: 10.1021/acs.jced.8b00115

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Below the room temperature measurements of solubilities in ester mixtures of CO₂ capture absorbents methyl formate, ethyl hexanoate and methyl formate plus hexanoate in the liquid phase. *Journal of Chemical Engineering Data*, 2019, 64 (1), 1-15. DOI: 10.1021/acs.jced.8b00115

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Estimated Solubility Method:

<https://www.doi.org/10.1016/j.jct.2018.07.021>

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