

Hexanoic acid

Other names:	1-Hexanoic acid
	1-Pentanecarboxylic acid
	Butylacetic acid
	CH3(CH2)4COOH
	Caproic acid
	Capronic acid
	Hexacid 698
	Hexoic acid
	Kyselina kapronova
	NSC 8266
	Pentane-1-carboxylic acid
	Pentanecarboxylic acid
	Pentiformic acid
	Pentylformic acid
	n-Caproic acid
	n-Hexanoic acid
	n-Hexoic acid
	n-Hexylic acid
Inchi:	InChI=1S/C6H12O2/c1-2-3-4-5-6(7)8/h2-5H2,1H3,(H,7,8)
InchiKey:	FUZZWVXGSFPDMH-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCCCC(=O)O
Mol. weight [g/mol]:	116.16
CAS:	142-62-1

Physical Properties

Property code	Value	Unit	Source
chl	-3494.29 ± 0.66	kJ/mol	NIST Webbook
chl	-3518.00	kJ/mol	NIST Webbook
chl	-3492.40 ± 0.60	kJ/mol	NIST Webbook
chl	-3490.40 ± 0.54	kJ/mol	NIST Webbook
chs	-3522.80	kJ/mol	NIST Webbook
gf	-266.10	kJ/mol	Joback Method
hf	-508.60 ± 2.30	kJ/mol	NIST Webbook
hf	-511.20 ± 1.50	kJ/mol	NIST Webbook
hf	-515.10 ± 1.10	kJ/mol	NIST Webbook
hf	-511.20 ± 1.50	kJ/mol	NIST Webbook

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hf	-515.10 ± 1.10	kJ/mol	NIST Webbook
hf	-512.50 ± 2.10	kJ/mol	NIST Webbook
hfl	-583.58 ± 0.75	kJ/mol	NIST Webbook
hfl	-581.80 ± 1.10	kJ/mol	NIST Webbook
hfl	-585.68 ± 0.54	kJ/mol	NIST Webbook
hfus	16.98	kJ/mol	Joback Method
hvap	69.20 ± 0.90	kJ/mol	NIST Webbook
hvap	71.00 ± 1.00	kJ/mol	NIST Webbook
hvap	73.20 ± 2.00	kJ/mol	NIST Webbook
hvap	73.20 ± 2.00	kJ/mol	NIST Webbook
hvap	71.30	kJ/mol	NIST Webbook
ie	10.12	eV	NIST Webbook
log10ws	-1.06		Aqueous Solubility Prediction Method
logp	1.651		Crippen Method
mcpvol	102.840	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=2)		KDB
pc	3154.44 ± 90.00	kPa	NIST Webbook
pc	3200.00 ± 100.00	kPa	NIST Webbook
pc	3377.00 ± 40.00	kPa	NIST Webbook
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ripol	1863.00	NIST Webbook
ripol	1830.00	NIST Webbook
ripol	1863.00	NIST Webbook
ripol	1850.00	NIST Webbook
ripol	1885.00	NIST Webbook
ripol	1863.00	NIST Webbook
ripol	1816.00	NIST Webbook
ripol	1876.00	NIST Webbook
ripol	1850.00	NIST Webbook
ripol	1852.00	NIST Webbook
ripol	1849.00	NIST Webbook
ripol	1826.00	NIST Webbook
ripol	1813.00	NIST Webbook
ripol	1821.00	NIST Webbook
ripol	1840.00	NIST Webbook
ripol	1870.00	NIST Webbook
ripol	1871.00	NIST Webbook
ripol	1848.00	NIST Webbook
ripol	1870.00	NIST Webbook
ripol	1845.00	NIST Webbook
ripol	1868.00	NIST Webbook
ripol	1854.00	NIST Webbook
ripol	1832.00	NIST Webbook
ripol	1836.00	NIST Webbook
ripol	1832.00	NIST Webbook
ripol	1871.00	NIST Webbook
ripol	1834.00	NIST Webbook
ripol	1852.00	NIST Webbook
ripol	1834.00	NIST Webbook
ripol	1839.00	NIST Webbook

ripol	1847.00		NIST Webbook
ripol	1870.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1822.00		NIST Webbook
tb	468.15 ± 5.00	K	NIST Webbook
tb	476.15 ± 5.00	K	NIST Webbook
tb	477.65 ± 4.00	K	NIST Webbook
tb	481.15 ± 4.00	K	NIST Webbook
tb	477.15 ± 3.00	K	NIST Webbook
tb	472.20 ± 1.50	K	NIST Webbook
tb	477.90 ± 1.50	K	NIST Webbook
tb	477.00 ± 3.00	K	NIST Webbook
tb	477.40 ± 1.50	K	NIST Webbook
tb	475.65 ± 3.00	K	NIST Webbook
tb	478.85 ± 1.50	K	NIST Webbook
tb	478.65 ± 3.00	K	NIST Webbook
tb	478.15 ± 2.00	K	NIST Webbook
tb	478.15 ± 2.00	K	NIST Webbook
tb	476.00 ± 6.00	K	NIST Webbook
tb	472.65 ± 3.00	K	NIST Webbook
tb	473.15 ± 3.00	K	NIST Webbook
tb	475.65 ± 3.00	K	NIST Webbook
tb	477.90 ± 1.50	K	NIST Webbook
tb	478.15 ± 2.00	K	NIST Webbook
tb	477.15 ± 2.00	K	NIST Webbook
tb	478.50 ± 0.20	K	NIST Webbook
tb	479.15 ± 2.00	K	NIST Webbook
tb	478.05 ± 1.00	K	NIST Webbook
tb	481.65 ± 3.00	K	NIST Webbook
tb	478.15 ± 2.00	K	NIST Webbook
tb	476.15 ± 3.00	K	NIST Webbook
tb	474.65 ± 3.00	K	NIST Webbook
tb	476.15 ± 2.00	K	NIST Webbook
tb	478.30 ± 0.70	K	NIST Webbook
tb	477.65 ± 2.00	K	NIST Webbook
tb	478.15 ± 2.00	K	NIST Webbook
tb	478.30 ± 0.50	K	NIST Webbook
tb	478.45 ± 0.50	K	NIST Webbook
tb	476.15 ± 2.00	K	NIST Webbook
tb	476.15 ± 2.00	K	NIST Webbook
tb	478.15 ± 2.00	K	NIST Webbook
tb	478.05 ± 0.50	K	NIST Webbook
tb	477.15 ± 3.00	K	NIST Webbook

tb	478.20	K	NIST Webbook
tb	475.70	K	NIST Webbook
tb	471.15 ± 5.00	K	NIST Webbook
tb	478.40	K	KDB
tc	663.00 ± 1.00	K	NIST Webbook
tc	655.10 ± 1.00	K	NIST Webbook
tc	662.00	K	KDB
tc	669.63 ± 3.00	K	NIST Webbook
tf	269.00 ± 4.00	K	NIST Webbook
tf	269.00 ± 1.50	K	NIST Webbook
tf	271.40 ± 1.50	K	NIST Webbook
tf	269.70 ± 0.05	K	NIST Webbook
tf	270.00	K	KDB
tf	269.90	K	Aqueous Solubility Prediction Method
tf	269.20 ± 0.50	K	NIST Webbook
tt	269.71	K	KDB
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.93	J/mol×K	654.09	Joback Method
cpg	232.52	J/mol×K	511.29	Joback Method
cpg	241.09	J/mol×K	539.85	Joback Method
cpg	249.31	J/mol×K	568.41	Joback Method
cpg	257.18	J/mol×K	596.97	Joback Method
cpg	264.72	J/mol×K	625.53	Joback Method
cpg	223.60	J/mol×K	482.73	Joback Method
cpl	225.10	J/mol×K	298.00	NIST Webbook
dvisc	0.0003313	Pa×s	446.96	Joback Method
dvisc	0.0011124	Pa×s	375.43	Joback Method
dvisc	0.0024680	Pa×s	339.66	Joback Method
dvisc	0.0066054	Pa×s	303.90	Joback Method
dvisc	0.0229887	Pa×s	268.13	Joback Method
dvisc	0.0002069	Pa×s	482.73	Joback Method
dvisc	0.0005759	Pa×s	411.20	Joback Method
hvapt	64.60	kJ/mol	367.00	NIST Webbook
hvapt	66.60	kJ/mol	411.50	NIST Webbook
hvapt	70.90	kJ/mol	271.00	NIST Webbook
hvapt	65.90	kJ/mol	411.00	NIST Webbook

hvapt	68.40 ± 0.90	kJ/mol	312.50	NIST Webbook
pvap	19.59	kPa	429.92	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	44.75	kPa	451.43	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	14.56	kPa	422.88	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	39.72	kPa	447.88	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	34.68	kPa	444.26	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid

pvap	29.64	kPa	440.03	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	24.63	kPa	435.62	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	9.52	kPa	413.40	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
rfi	1.41500		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
rfi	1.41470		298.15	Liquid-Liquid Equilibria for Ternary Mixtures of gamma-Valerolactone + n-Tetradecane + (Butanoic Acid or Hexanoic Acid or Methyl Myristate) at 298.15 K
rhoI	893.10	kg/m3	332.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K

rhoI	825.30	kg/m3	408.30	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	806.50	kg/m3	428.30	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	922.06	kg/m3	298.15	Excess molar enthalpies of binary systems containing 2-octanone, hexanoic acid, or octanoic acid at T = 298.15 K
rhoI	923.07	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
rhoI	926.00	kg/m3	294.50	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	910.50	kg/m3	312.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	875.80	kg/m3	352.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K

rhoI	843.50	kg/m3	388.40	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhoI	861.70	kg/m3	368.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
srf	0.03	N/m	308.15	Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Carboxylic Acids
srf	0.03	N/m	303.15	Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Carboxylic Acids
srf	0.03	N/m	298.15	Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Carboxylic Acids
srf	0.03	N/m	293.15	Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Carboxylic Acids

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53785e+01
Coeff. B	-4.07436e+03
Coeff. C	-9.83480e+01

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid 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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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