

# Hexanoic acid, 2-ethyl-

<b>Other names:</b>	2-Butylbutanoic acid 2-Ethyl-1-hexanoic acid 2-Ethylcaproic acid 2-Ethylcapronic acid 2-Ethylhexanoic acid 2-Ethylhexoic acid 3-Heptanecarboxylic acid Butylethylacetic acid Ethylhexanoic acid Ethylhexoic acid Kyselina 2-ethylkapronova Kyselina heptan-3-karboxylova NSC 8881 «alpha»-Ethylcaproic acid «alpha»-Ethylhexanoic acid Â«alphaÂ»-Ethylcaproic acid Â«alphaÂ»-Ethylhexanoic acid
<b>Inchi:</b>	InChI=1S/C8H16O2/c1-3-5-6-7(4-2)8(9)10/h7H,3-6H2,1-2H3,(H,9,10)
<b>InchiKey:</b>	OBETXYAYXDNJHR-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O2
<b>SMILES:</b>	CCCCCC(CC)C(=O)O
<b>Mol. weight [g/mol]:</b>	144.21
<b>CAS:</b>	149-57-5

## Physical Properties

Property code	Value	Unit	Source
chl	-4799.60 ± 1.70	kJ/mol	NIST Webbook
gf	-251.70	kJ/mol	Joback Method
hf	-559.50 ± 2.10	kJ/mol	NIST Webbook
hfl	-635.10 ± 2.00	kJ/mol	NIST Webbook
hfus	18.64	kJ/mol	Joback Method
hvap	76.30 ± 0.90	kJ/mol	NIST Webbook
hvap	75.60 ± 0.42	kJ/mol	NIST Webbook
hvap	75.60 ± 0.50	kJ/mol	NIST Webbook
log10ws	-2.03		Crippen Method
logp	2.287		Crippen Method
mcvol	131.020	ml/mol	McGowan Method

pc	2778.00 ± 40.00	kPa	NIST Webbook
pc	2780.00 ± 300.00	kPa	NIST Webbook
rhoc	272.56 ± 5.77	kg/m3	NIST Webbook
rhoc	260.01 ± 14.42	kg/m3	NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	180.80		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1085.19		NIST Webbook
rinpol	1116.70		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	180.80		NIST Webbook
ripol	1962.50		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1918.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1933.00		NIST Webbook
ripol	1937.00		NIST Webbook

ripol	1965.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1962.50		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1928.00		NIST Webbook
ripol	1969.00		NIST Webbook
tb	500.15	K	NIST Webbook
tb	501.20	K	NIST Webbook
tc	673.60 ± 1.20	K	NIST Webbook
tc	674.60 ± 0.80	K	NIST Webbook
tc	675.00 ± 5.00	K	NIST Webbook
tf	154.75	K	NIST Webbook
vc	0.502	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.66	J/molxK	700.14	Joback Method
cpg	360.77	J/molxK	671.46	Joback Method
cpg	351.46	J/molxK	642.78	Joback Method
cpg	341.71	J/molxK	614.10	Joback Method
cpg	331.52	J/molxK	585.41	Joback Method
cpg	320.87	J/molxK	556.73	Joback Method
cpg	309.75	J/molxK	528.05	Joback Method
dvisc	0.0284980	Paxs	275.67	Joback Method
dvisc	0.0001397	Paxs	528.05	Joback Method
dvisc	0.0002310	Paxs	485.99	Joback Method
dvisc	0.0004201	Paxs	443.92	Joback Method
dvisc	0.0008658	Paxs	401.86	Joback Method
dvisc	0.0021132	Paxs	359.80	Joback Method
dvisc	0.0065326	Paxs	317.73	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58601e+01
Coeff. B	-4.63462e+03
Coeff. C	-8.89300e+01
Temperature range (K), min.	386.55
Temperature range (K), max.	528.29

## Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C149575&Units=SI>

The Yaws Handbook of Vapor

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Pressure:

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

The co-solubility of 2-ethylhexanoic

<https://www.doi.org/10.1016/j.fluid.2005.09.023>

acid and some liquid alcohols in

Supercritical carbon dioxide,

Solubility of 2-Ethylhexanol,

2-Ethylhexanoic Acid, and Their

Mixtures in Supercritical Carbon

Dioxide:

McGowan Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

## Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rhoc:</b>	Critical density
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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