Hexanoic acid, 2-ethyl-

Other names:	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
Inchi:	InChI=1S/C8H16O2/c1-3-5-6-7(4-2)8(9)10/h7H,3-6H2,1-2H3,(H,9,10)
InchiKey:	OBETXYAYXDNJHR-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCC(CC)C(=O)O
Mol. weight [g/mol]:	144.21
CAS:	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	75.60 ± 0.42	kJ/mol	NIST Webbook
hvap	76.30 ± 0.90	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	2780.00 ± 300.00	kPa	NIST Webbook
pc	2778.00 ± 40.00	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	1139.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	180.80		NIST Webbook
rinpol	180.80		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1116.70		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1085.19		NIST Webbook
ripol	1962.50		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1968.00		NIST Webbook

ripol	1968.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1937.00		NIST Webbook
ripol	1933.00		NIST Webbook
ripol	1928.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1918.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1962.50		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1969.00		NIST Webbook
tb	500.15	K	NIST Webbook
tb	501.20	K	NIST Webbook
tc	675.00 ± 5.00	K	NIST Webbook
tc	673.60 ± 1.20	K	NIST Webbook
tc	674.60 ± 0.80	K	NIST Webbook
tf	154.75	K	NIST Webbook
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

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

hvapt	61.80	kJ/mol	451.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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 Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The co-solubility of 2-ethylhexanoic acid and some liquid alcohols in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2005.09.023
Solubility of 2-Ethyl-1-hexanol, 2-Ethylhexanoic Acid, and Their Mixtures in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je020074l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan 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

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