

# Hexanoic acid, 3-oxo-, ethyl ester

<b>Other names:</b>	Ethyl «alpha»-butyrylacetate Ethyl butyroacetate Ethyl butyrylacetate Ethyl 3-oxohexanoate 3-Keto-n-hexanoic acid ethyl ester
<b>Inchi:</b>	InChI=1S/C8H14O3/c1-3-5-7(9)6-8(10)11-4-2/h3-6H2,1-2H3
<b>InchiKey:</b>	KQWWVLVLVYYYDT-UHFFFAOYSA-N
<b>Formula:</b>	C8H14O3
<b>SMILES:</b>	CCCC(=O)CC(=O)OCC
<b>Mol. weight [g/mol]:</b>	158.19
<b>CAS:</b>	3249-68-1

## Physical Properties

Property code	Value	Unit	Source
gf	-346.36	kJ/mol	Joback Method
hf	-565.83	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	49.30	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.309		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
tb	512.60	K	Joback Method
tc	697.35	K	Joback Method
tf	302.01	K	Joback Method
vc	0.513	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.67	J/molxK	512.60	Joback Method
cpg	351.97	J/molxK	666.56	Joback Method
cpg	342.23	J/molxK	635.77	Joback Method
cpg	332.03	J/molxK	604.98	Joback Method

cpg	321.37	J/molxK	574.18	Joback Method
cpg	310.25	J/molxK	543.39	Joback Method
cpg	361.25	J/molxK	697.35	Joback Method
dvisc	0.0002790	Paxs	512.60	Joback Method
dvisc	0.0003549	Paxs	477.50	Joback Method
dvisc	0.0004690	Paxs	442.40	Joback Method
dvisc	0.0006504	Paxs	407.31	Joback Method
dvisc	0.0009592	Paxs	372.21	Joback Method
dvisc	0.0015339	Paxs	337.11	Joback Method
dvisc	0.0027356	Paxs	302.01	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.20	K	2.90	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3249681&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3249681&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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