

# 2-Butenoic acid, 3-ethoxy-, ethyl ester

<b>Other names:</b>	Crotonic acid, 3-ethoxy-, ethyl ester Ethyl 3-ethoxy-2-butenolate Ethyl 3-ethoxycrotonate 3-Ethoxy-2-butenoic acid ethyl ester Ethyl «beta»-ethoxy-crotonate Ethyl 3-ethoxybut-2-enoate
<b>Inchi:</b>	InChI=1S/C8H14O3/c1-4-10-7(3)6-8(9)11-5-2/h6H,4-5H2,1-3H3/b7-6+
<b>InchiKey:</b>	ZOCYCSPSSNMXBU-VOTSOKGWSA-N
<b>Formula:</b>	C8H14O3
<b>SMILES:</b>	CCOC(=O)C=C(C)OCC
<b>Mol. weight [g/mol]:</b>	158.19
<b>CAS:</b>	998-91-4

## Physical Properties

Property code	Value	Unit	Source
chl	-4501.65	kJ/mol	NIST Webbook
gf	-250.77	kJ/mol	Joback Method
hf	-478.04	kJ/mol	Joback Method
hfus	19.34	kJ/mol	Joback Method
hvap	45.01	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.490		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	485.19	K	Joback Method
tc	671.03	K	Joback Method
tf	255.27	K	Joback Method
vc	0.506	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.67	J/molxK	485.19	Joback Method
cpg	298.54	J/molxK	516.16	Joback Method

cpg	309.96	J/mol×K	547.14	Joback Method
cpg	320.93	J/mol×K	578.11	Joback Method
cpg	331.46	J/mol×K	609.09	Joback Method
cpg	341.54	J/mol×K	640.06	Joback Method
cpg	351.19	J/mol×K	671.03	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.50 ± 1.50	K	2.70	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C998914&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C998914&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>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<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

**vc:** Critical Volume

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