

# (Z)-Ethyl 2-methylbut-2-enoate

<b>Inchi:</b>	InChI=1S/C7H12O2/c1-4-6(3)7(8)9-5-2/h4H,5H2,1-3H3/b6-4-
<b>InchiKey:</b>	OAPHLAAOJMTMLY-XQRVVYSFSA-N
<b>Formula:</b>	C7H12O2
<b>SMILES:</b>	CC=C(C)C(=O)OCC
<b>Mol. weight [g/mol]:</b>	128.17
<b>CAS:</b>	16509-44-7

## Physical Properties

Property code	Value	Unit	Source
gf	-154.19	kJ/mol	Joback Method
hf	-325.18	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	40.37	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	899.30		NIST Webbook
tb	439.89	K	Joback Method
tc	628.49	K	Joback Method
tf	221.77	K	Joback Method
vc	0.432	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.62	J/molxK	439.89	Joback Method
cpg	233.55	J/molxK	471.32	Joback Method
cpg	244.02	J/molxK	502.76	Joback Method
cpg	254.05	J/molxK	534.19	Joback Method
cpg	263.64	J/molxK	565.63	Joback Method
cpg	272.80	J/molxK	597.06	Joback Method
cpg	281.54	J/molxK	628.49	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16509447&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16509447&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<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>rinpola:</b>	Non-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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