

# (Z)-2-Pentenoic acid ethyl ester

**Inchi:** InChI=1S/C7H12O2/c1-3-5-6-7(8)9-4-2/h5-6H,3-4H2,1-2H3/b6-5-  
**InchiKey:** AGMKVZDPATUSMS-WAYWQWQTSA-N  
**Formula:** C7H12O2  
**SMILES:** CCC=CC(=O)OCC  
**Mol. weight [g/mol]:** 128.17  
**CAS:** 27805-84-1

## Physical Properties

Property code	Value	Unit	Source
chl	-4029.00 ± 3.00	kJ/mol	NIST Webbook
gf	-145.64	kJ/mol	Joback Method
hf	-395.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-441.00 ± 3.00	kJ/mol	NIST Webbook
hfus	16.88	kJ/mol	Joback Method
hvap	46.00	kJ/mol	NIST Webbook
hvap	46.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	440.01	K	Joback Method
tc	625.03	K	Joback Method
tf	235.73	K	Joback Method
vc	0.431	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.68	J/molxK	440.01	Joback Method
cpg	233.44	J/molxK	470.85	Joback Method
cpg	243.76	J/molxK	501.68	Joback Method
cpg	253.64	J/molxK	532.52	Joback Method
cpg	263.10	J/molxK	563.36	Joback Method
cpg	272.15	J/molxK	594.20	Joback Method

cpg	280.80	J/mol×K	625.03	Joback Method
dvisc	0.0029377	Paxs	235.73	Joback Method
dvisc	0.0014537	Paxs	269.78	Joback Method
dvisc	0.0008422	Paxs	303.82	Joback Method
dvisc	0.0005447	Paxs	337.87	Joback Method
dvisc	0.0003815	Paxs	371.92	Joback Method
dvisc	0.0002837	Paxs	405.96	Joback Method
dvisc	0.0002208	Paxs	440.01	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C27805841&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27805841&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>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase 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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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