

# CH<sub>3</sub>C(OCH<sub>3</sub>)=CHCOOCH<sub>3</sub>

<b>Inchi:</b>	InChI=1S/C6H10O3/c1-5(8-2)4-6(7)9-3/h4H,1-3H3
<b>InchiKey:</b>	RJSHZZLJYZOHRU-UHFFFAOYSA-N
<b>Formula:</b>	C6H10O3
<b>SMILES:</b>	COC(=O)C=C(C)OC
<b>Mol. weight [g/mol]:</b>	130.14
<b>CAS:</b>	22157-30-8

## Physical Properties

Property code	Value	Unit	Source
affp	916.80	kJ/mol	NIST Webbook
basg	885.80	kJ/mol	NIST Webbook
gf	-267.61	kJ/mol	Joback Method
hf	-436.76	kJ/mol	Joback Method
hfus	14.16	kJ/mol	Joback Method
hvap	40.55	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.710		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	439.43	K	Joback Method
tc	629.13	K	Joback Method
tf	232.73	K	Joback Method
vc	0.395	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.63	J/mol×K	439.43	Joback Method
cpg	215.07	J/mol×K	471.05	Joback Method
cpg	224.20	J/mol×K	502.66	Joback Method
cpg	233.00	J/mol×K	534.28	Joback Method
cpg	241.48	J/mol×K	565.90	Joback Method
cpg	249.63	J/mol×K	597.52	Joback Method
cpg	257.46	J/mol×K	629.13	Joback Method

# Sources

<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=C22157308&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22157308&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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