

# 6-Methyl - 2,4-dioxo-5- heptenoic acid, ethyl ester

Inchi:	InChI=1S/C10H14O4/c1-4-14-10(13)9(12)6-8(11)5-7(2)3/h5H,4,6H2,1-3H3
InchiKey:	JNJLOBHXZALHNZ-UHFFFAOYSA-N
Formula:	C10H14O4
SMILES:	CCOC(=O)C(=O)CC(=O)C=C(C)C
Mol. weight [g/mol]:	198.22
CAS:	92736-02-2

## Physical Properties

Property code	Value	Unit	Source
gf	-386.77	kJ/mol	Joback Method
hf	-612.26	kJ/mol	Joback Method
hfus	26.53	kJ/mol	Joback Method
hvap	60.54	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.044		Crippen Method
mcvol	158.040	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
tb	616.27	K	Joback Method
tc	815.39	K	Joback Method
tf	355.44	K	Joback Method
vc	0.613	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.66	J/molxK	616.27	Joback Method
cpg	399.63	J/molxK	649.46	Joback Method
cpg	410.96	J/molxK	682.64	Joback Method
cpg	421.67	J/molxK	715.83	Joback Method
cpg	431.76	J/molxK	749.02	Joback Method
cpg	441.25	J/molxK	782.20	Joback Method
cpg	450.17	J/molxK	815.39	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C92736022&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92736022&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>
<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>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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