

# Isobutyric acid, isobutenyl ester

<b>Inchi:</b>	InChI=1S/C8H14O2/c1-6(2)5-10-8(9)7(3)4/h5,7H,1-4H3
<b>InchiKey:</b>	RQOBTHQSTIYLCE-UHFFFAOYSA-N
<b>Formula:</b>	C8H14O2
<b>SMILES:</b>	CC(C)=COC(=O)C(C)C
<b>Mol. weight [g/mol]:</b>	142.20
<b>CAS:</b>	86123-20-8

## Physical Properties

Property code	Value	Unit	Source
gf	-148.21	kJ/mol	Joback Method
hf	-351.10	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	42.21	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.109		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	462.33	K	Joback Method
tc	653.28	K	Joback Method
tf	218.04	K	Joback Method
vc	0.482	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.35	J/molxK	462.33	Joback Method
cpg	275.79	J/molxK	494.15	Joback Method
cpg	287.69	J/molxK	525.98	Joback Method
cpg	299.05	J/molxK	557.80	Joback Method
cpg	309.90	J/molxK	589.63	Joback Method
cpg	320.24	J/molxK	621.45	Joback Method
cpg	330.09	J/molxK	653.28	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=C86123208&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C86123208&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>

# 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>mccvol:</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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