

# Propanoic acid, 2-methyl-, 3-methyl-2-butenyl ester

<b>Other names:</b>	Prenyl isobutyrate 3-methylbut-2-enyl isobutyrate
<b>Inchi:</b>	InChI=1S/C9H16O2/c1-7(2)5-6-11-9(10)8(3)4/h5,8H,6H2,1-4H3
<b>InchiKey:</b>	YSJHMPXIMIOXGU-UHFFFAOYSA-N
<b>Formula:</b>	C9H16O2
<b>SMILES:</b>	CC(C)=CCOC(=O)C(C)C
<b>Mol. weight [g/mol]:</b>	156.22
<b>CAS:</b>	76649-23-5

## Physical Properties

Property code	Value	Unit	Source
gf	-139.79	kJ/mol	Joback Method
hf	-371.74	kJ/mol	Joback Method
hfus	17.22	kJ/mol	Joback Method
hvap	44.43	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.152		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1053.00		NIST Webbook
rinpol	1053.00		NIST Webbook
tb	485.21	K	Joback Method
tc	674.06	K	Joback Method
tf	229.31	K	Joback Method
vc	0.538	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.09	J/molxK	485.21	Joback Method
cpg	319.56	J/molxK	516.68	Joback Method
cpg	332.44	J/molxK	548.16	Joback Method
cpg	344.74	J/molxK	579.63	Joback Method
cpg	356.48	J/molxK	611.11	Joback Method

cpg	367.66	J/mol×K	642.58	Joback Method
cpg	378.31	J/mol×K	674.06	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=C76649235&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C76649235&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>hvac:</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>rinpol:</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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