

# butanoic acid, 3-methyl-3Z-hexen-1-yl ester

<b>Inchi:</b>	InChI=1S/C11H20O2/c1-4-6-10(3)8-9-13-11(12)7-5-2/h6H,4-5,7-9H2,1-3H3/b10-6-
<b>InchiKey:</b>	SMJVHJPBTMEGCQ-POHAHGRESA-N
<b>Formula:</b>	C11H20O2
<b>SMILES:</b>	CCC=C(C)CCOC(=O)CCC
<b>Mol. weight [g/mol]:</b>	184.28

## Physical Properties

Property code	Value	Unit	Source
gf	-120.51	kJ/mol	Joback Method
hf	-407.74	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	49.27	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinsol	1237.00		NIST Webbook
tb	531.41	K	Joback Method
tc	712.45	K	Joback Method
tf	266.85	K	Joback Method
vc	0.656	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.17	J/mol×K	531.41	Joback Method
cpg	412.00	J/mol×K	561.58	Joback Method
cpg	426.18	J/mol×K	591.76	Joback Method
cpg	439.73	J/mol×K	621.93	Joback Method
cpg	452.68	J/mol×K	652.10	Joback Method
cpg	465.03	J/mol×K	682.28	Joback Method
cpg	476.80	J/mol×K	712.45	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=R395710&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R395710&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>

# 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>mccol:</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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