

# Butanoic acid, 2,2-dimethylpropyl ester

<b>Inchi:</b>	InChI=1S/C9H18O2/c1-5-6-8(10)11-7-9(2,3)4/h5-7H2,1-4H3
<b>InchiKey:</b>	BLTRSYBDPNEMNK-UHFFFAOYSA-N
<b>Formula:</b>	C9H18O2
<b>SMILES:</b>	CCCC(=O)OCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	158.24
<b>CAS:</b>	23361-69-5

## Physical Properties

Property code	Value	Unit	Source
gf	-206.18	kJ/mol	Joback Method
hf	-482.64	kJ/mol	Joback Method
hfus	14.44	kJ/mol	Joback Method
hvap	43.49	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
tb	478.38	K	Joback Method
tc	662.57	K	Joback Method
tf	265.77	K	Joback Method
vc	0.552	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.67	J/molxK	478.38	Joback Method
cpg	391.10	J/molxK	631.87	Joback Method
cpg	379.26	J/molxK	601.18	Joback Method
cpg	366.81	J/molxK	570.48	Joback Method
cpg	353.74	J/molxK	539.78	Joback Method
cpg	340.03	J/molxK	509.08	Joback Method
cpg	402.36	J/molxK	662.57	Joback Method
dvisc	0.0002372	Paxs	478.38	Joback Method
dvisc	0.0003187	Paxs	442.94	Joback Method

dvisc	0.0004508	Paxs	407.51	Joback Method
dvisc	0.0006812	Paxs	372.07	Joback Method
dvisc	0.0011229	Paxs	336.64	Joback Method
dvisc	0.0020820	Paxs	301.20	Joback Method
dvisc	0.0045510	Paxs	265.77	Joback Method

## Sources

<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>
<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=C23361695&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23361695&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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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