

# Succinic acid, monochloride, 3-methylbutyl ester

Inchi:	InChI=1S/C9H15ClO3/c1-7(2)5-6-13-9(12)4-3-8(10)11/h7H,3-6H2,1-2H3
InchiKey:	NVHUMKDRBJLIC-UHFFFAOYSA-N
Formula:	C9H15ClO3
SMILES:	CC(C)CCOC(=O)CCC(=O)Cl
Mol. weight [g/mol]:	206.67

## Physical Properties

Property code	Value	Unit	Source
gf	-352.31	kJ/mol	Joback Method
hf	-607.49	kJ/mol	Joback Method
hfus	24.13	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.121		Crippen Method
mcvol	158.920	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinsol	1308.00		NIST Webbook
tb	572.47	K	Joback Method
tc	763.57	K	Joback Method
tf	328.20	K	Joback Method
vc	0.613	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.99	J/molxK	572.47	Joback Method
cpg	383.21	J/molxK	604.32	Joback Method
cpg	394.86	J/molxK	636.17	Joback Method
cpg	405.94	J/molxK	668.02	Joback Method
cpg	416.45	J/molxK	699.87	Joback Method
cpg	426.41	J/molxK	731.72	Joback Method
cpg	435.82	J/molxK	763.57	Joback Method
dvisc	0.0030874	Paxs	328.20	Joback Method
dvisc	0.0015857	Paxs	368.91	Joback Method

dvisc	0.0009298	Paxs	409.62	Joback Method
dvisc	0.0006004	Paxs	450.34	Joback Method
dvisc	0.0004169	Paxs	491.05	Joback Method
dvisc	0.0003061	Paxs	531.76	Joback Method
dvisc	0.0002348	Paxs	572.47	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=U349262&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349262&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>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>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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