

# Glutaric acid, monochloride, 3-oxobut-2-yl ester

Inchi:	InChI=1S/C9H13ClO4/c1-6(11)7(2)14-9(13)5-3-4-8(10)12/h7H,3-5H2,1-2H3
InchiKey:	VZGGHTAJHHLUOG-UHFFFAOYSA-N
Formula:	C9H13ClO4
SMILES:	CC(=O)C(C)OC(=O)CCCC(=O)Cl
Mol. weight [g/mol]:	220.65

## Physical Properties

Property code	Value	Unit	Source
gf	-481.23	kJ/mol	Joback Method
hf	-720.07	kJ/mol	Joback Method
hfus	25.73	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.443		Crippen Method
mvol	160.490	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
tb	626.34	K	Joback Method
tc	824.94	K	Joback Method
tf	378.13	K	Joback Method
vc	0.619	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.26	J/molxK	626.34	Joback Method
cpg	397.44	J/molxK	659.44	Joback Method
cpg	408.02	J/molxK	692.54	Joback Method
cpg	417.98	J/molxK	725.64	Joback Method
cpg	427.35	J/molxK	758.74	Joback Method
cpg	436.13	J/molxK	791.84	Joback Method
cpg	444.32	J/molxK	824.94	Joback Method
dvisc	0.0024489	Paxs	378.13	Joback Method

dvisc	0.0013698	Paxs	419.50	Joback Method
dvisc	0.0008505	Paxs	460.87	Joback Method
dvisc	0.0005711	Paxs	502.24	Joback Method
dvisc	0.0004075	Paxs	543.60	Joback Method
dvisc	0.0003050	Paxs	584.97	Joback Method
dvisc	0.0002372	Paxs	626.34	Joback Method

## Sources

<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=U359716&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359716&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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