

# Glutaric acid, 2-methylpent-3-yl 3-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C17H23ClO4/c1-4-15(12(2)3)22-17(20)10-6-9-16(19)21-14-8-5-7-13(18)11-14
<b>InchiKey:</b>	SYFOTMZOJRHQN-UHFFFAOYSA-N
<b>Formula:</b>	C17H23ClO4
<b>SMILES:</b>	CCC(OC(=O)CCCC(=O)Oc1cccc(Cl)c1)C(C)C
<b>Mol. weight [g/mol]:</b>	326.81

## Physical Properties

Property code	Value	Unit	Source
gf	-289.61	kJ/mol	Joback Method
hf	-685.05	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	78.30	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.393		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
tb	809.15	K	Joback Method
tc	1018.80	K	Joback Method
tf	464.53	K	Joback Method
vc	0.965	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.45	J/molxK	809.15	Joback Method
cpg	747.08	J/molxK	844.09	Joback Method
cpg	760.60	J/molxK	879.03	Joback Method
cpg	773.05	J/molxK	913.98	Joback Method
cpg	784.43	J/molxK	948.92	Joback Method
cpg	794.77	J/molxK	983.86	Joback Method
cpg	804.08	J/molxK	1018.80	Joback Method
dvisc	0.0008514	Paxs	464.53	Joback Method

dvisc	0.0004307	Paxs	521.97	Joback Method
dvisc	0.0002494	Paxs	579.40	Joback Method
dvisc	0.0001594	Paxs	636.84	Joback Method
dvisc	0.0001097	Paxs	694.28	Joback Method
dvisc	0.0000799	Paxs	751.71	Joback Method
dvisc	0.0000609	Paxs	809.15	Joback Method

## Sources

<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=U390458&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390458&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>
<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>

## 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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