

# Glutaric acid, monochloride, 2-heptyl ester

<b>Inchi:</b>	InChI=1S/C12H21ClO3/c1-3-4-5-7-10(2)16-12(15)9-6-8-11(13)14/h10H,3-9H2,1-2H3
<b>InchiKey:</b>	KRYMKWMJARZPGE-UHFFFAOYSA-N
<b>Formula:</b>	C12H21ClO3
<b>SMILES:</b>	CCCCC(C)OC(=O)CCCC(=O)Cl
<b>Mol. weight [g/mol]:</b>	248.75

## Physical Properties

Property code	Value	Unit	Source
gf	-327.05	kJ/mol	Joback Method
hf	-669.41	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.434		Crippen Method
mcvol	201.190	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpola	1638.00		NIST Webbook
tb	641.11	K	Joback Method
tc	826.30	K	Joback Method
tf	362.01	K	Joback Method
vc	0.780	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.93	J/molxK	641.11	Joback Method
cpg	533.20	J/molxK	671.97	Joback Method
cpg	546.76	J/molxK	702.84	Joback Method
cpg	559.64	J/molxK	733.70	Joback Method
cpg	571.83	J/molxK	764.57	Joback Method
cpg	583.36	J/molxK	795.43	Joback Method
cpg	594.23	J/molxK	826.30	Joback Method
dvisc	0.0025398	Paxs	362.01	Joback Method
dvisc	0.0012461	Paxs	408.53	Joback Method

dvisc	0.0007072	Paxs	455.04	Joback Method
dvisc	0.0004458	Paxs	501.56	Joback Method
dvisc	0.0003039	Paxs	548.08	Joback Method
dvisc	0.0002200	Paxs	594.59	Joback Method
dvisc	0.0001669	Paxs	641.11	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=U359580&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359580&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>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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