

# Glutaric acid, monochloride, 3-hexyl ester

<b>Inchi:</b>	InChI=1S/C11H19ClO3/c1-3-6-9(4-2)15-11(14)8-5-7-10(12)13/h9H,3-8H2,1-2H3
<b>InchiKey:</b>	ARCXVZMTSNLPNV-UHFFFAOYSA-N
<b>Formula:</b>	C11H19ClO3
<b>SMILES:</b>	CCCC(CC)OC(=O)CCCC(=O)Cl
<b>Mol. weight [g/mol]:</b>	234.72

## Physical Properties

Property code	Value	Unit	Source
gf	-335.47	kJ/mol	Joback Method
hf	-648.77	kJ/mol	Joback Method
hfus	29.31	kJ/mol	Joback Method
hvap	59.98	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.044		Crippen Method
mcvol	187.100	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinqol	1528.00		NIST Webbook
tb	618.23	K	Joback Method
tc	805.12	K	Joback Method
tf	350.74	K	Joback Method
vc	0.725	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.05	J/molxK	618.23	Joback Method
cpg	481.72	J/molxK	649.38	Joback Method
cpg	494.73	J/molxK	680.53	Joback Method
cpg	507.08	J/molxK	711.67	Joback Method
cpg	518.79	J/molxK	742.82	Joback Method
cpg	529.86	J/molxK	773.97	Joback Method
cpg	540.31	J/molxK	805.12	Joback Method
dvisc	0.0027334	Paxs	350.74	Joback Method
dvisc	0.0013605	Paxs	395.32	Joback Method

dvisc	0.0007801	Paxs	439.90	Joback Method
dvisc	0.0004955	Paxs	484.49	Joback Method
dvisc	0.0003397	Paxs	529.07	Joback Method
dvisc	0.0002470	Paxs	573.65	Joback Method
dvisc	0.0001880	Paxs	618.23	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=U359560&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359560&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>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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