

# Glutaric acid, 3-chlorobenzyl ethyl ester

<b>Inchi:</b>	InChI=1S/C14H17ClO4/c1-2-18-13(16)7-4-8-14(17)19-10-11-5-3-6-12(15)9-11/h3,5-6,9H
<b>InchiKey:</b>	VZIWWSGZBNMUFI-UHFFFAOYSA-N
<b>Formula:</b>	C14H17ClO4
<b>SMILES:</b>	CCOC(=O)CCCC(=O)OCc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	284.74

## Physical Properties

Property code	Value	Unit	Source
gf	-309.99	kJ/mol	Joback Method
hf	-612.57	kJ/mol	Joback Method
hfus	35.44	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.117		Crippen Method
mcvol	211.480	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpola	2253.00		NIST Webbook
tb	741.39	K	Joback Method
tc	950.76	K	Joback Method
tf	460.72	K	Joback Method
vc	0.808	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.99	J/molxK	741.39	Joback Method
cpg	579.31	J/molxK	776.28	Joback Method
cpg	591.71	J/molxK	811.18	Joback Method
cpg	603.21	J/molxK	846.07	Joback Method
cpg	613.81	J/molxK	880.97	Joback Method
cpg	623.52	J/molxK	915.86	Joback Method
cpg	632.35	J/molxK	950.76	Joback Method
dvisc	0.0008524	Paxs	460.72	Joback Method
dvisc	0.0005150	Paxs	507.50	Joback Method

dvisc	0.0003387	Paxs	554.28	Joback Method
dvisc	0.0002378	Paxs	601.06	Joback Method
dvisc	0.0001757	Paxs	647.83	Joback Method
dvisc	0.0001353	Paxs	694.61	Joback Method
dvisc	0.0001076	Paxs	741.39	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=U377588&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377588&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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