

# Glutaric acid, (2-chlorocyclohexyl)methyl cyclohexylmethyl ester

**Inchi:** InChI=1S/C19H31ClO4/c20-17-10-5-4-9-16(17)14-24-19(22)12-6-11-18(21)23-13-15-7-2  
**InchiKey:** UOLMRCUIZDOSIQ-UHFFFAOYSA-N  
**Formula:** C19H31ClO4  
**SMILES:** O=C(CCCC(=O)OCC1CCCCC1Cl)OCC1CCCCC1  
**Mol. weight [g/mol]:** 358.90

## Physical Properties

Property code	Value	Unit	Source
gf	-329.48	kJ/mol	Joback Method
hf	-852.53	kJ/mol	Joback Method
hfus	39.48	kJ/mol	Joback Method
hvap	81.13	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.621		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinpol	2698.00		NIST Webbook
tb	858.56	K	Joback Method
tc	1077.46	K	Joback Method
tf	488.65	K	Joback Method
vc	1.062	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.51	J/molxK	858.56	Joback Method
cpg	955.24	J/molxK	895.04	Joback Method
cpg	972.26	J/molxK	931.53	Joback Method
cpg	987.60	J/molxK	968.01	Joback Method
cpg	1001.27	J/molxK	1004.49	Joback Method
cpg	1013.31	J/molxK	1040.97	Joback Method
cpg	1023.73	J/molxK	1077.46	Joback Method
dvisc	0.0010356	Paxs	488.65	Joback Method
dvisc	0.0005196	Paxs	550.30	Joback Method

dvisc	0.0002996	Paxs	611.95	Joback Method
dvisc	0.0001910	Paxs	673.61	Joback Method
dvisc	0.0001314	Paxs	735.26	Joback Method
dvisc	0.0000957	Paxs	796.91	Joback Method
dvisc	0.0000730	Paxs	858.56	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=U405448&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405448&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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