

# Glutaric acid, (cyclohex-3-enyl)methyl 3-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C18H21ClO4/c19-15-8-4-9-16(12-15)23-18(21)11-5-10-17(20)22-13-14-6-2-1-3
<b>InchiKey:</b>	PNKLFKCVHHQRV-UHFFFAOYSA-N
<b>Formula:</b>	C18H21ClO4
<b>SMILES:</b>	O=C(CCCC(=O)Oc1cccc(Cl)c1)OCC1CC=CCC1
<b>Mol. weight [g/mol]:</b>	336.81

## Physical Properties

Property code	Value	Unit	Source
gf	-221.90	kJ/mol	Joback Method
hf	-583.03	kJ/mol	Joback Method
hfus	38.86	kJ/mol	Joback Method
hvap	82.02	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.315		Crippen Method
mcvol	252.680	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
tb	851.62	K	Joback Method
tc	1079.39	K	Joback Method
tf	513.94	K	Joback Method
vc	0.952	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.97	J/molxK	851.62	Joback Method
cpg	813.67	J/molxK	1041.43	Joback Method
cpg	804.39	J/molxK	1003.47	Joback Method
cpg	793.82	J/molxK	965.50	Joback Method
cpg	781.91	J/molxK	927.54	Joback Method
cpg	768.64	J/molxK	889.58	Joback Method
cpg	821.67	J/molxK	1079.39	Joback Method
dvisc	0.0000703	Paxs	851.62	Joback Method
dvisc	0.0000897	Paxs	795.34	Joback Method
dvisc	0.0001187	Paxs	739.06	Joback Method

dvisc	0.0001644	Paxs	682.78	Joback Method
dvisc	0.0002415	Paxs	626.50	Joback Method
dvisc	0.0003829	Paxs	570.22	Joback Method
dvisc	0.0006713	Paxs	513.94	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=U405531&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405531&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>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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