

# Glutaric acid, hexa-1,5-dien-3-yl 3-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C17H19ClO4/c1-3-7-14(4-2)21-16(19)10-6-11-17(20)22-15-9-5-8-13(18)12-15
<b>InchiKey:</b>	PEYOTWPERNCBBX-UHFFFAOYSA-N
<b>Formula:</b>	C17H19ClO4
<b>SMILES:</b>	<chem>C=CCC(C=C)OC(=O)CCCC(=O)Oc1cccc(Cl)c1</chem>
<b>Mol. weight [g/mol]:</b>	322.78

## Physical Properties

Property code	Value	Unit	Source
gf	-111.49	kJ/mol	Joback Method
hf	-428.91	kJ/mol	Joback Method
hfus	37.13	kJ/mol	Joback Method
hvap	77.34	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.090		Crippen Method
mcvol	245.150	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2194.00		NIST Webbook
rinpol	2194.00		NIST Webbook
tb	802.95	K	Joback Method
tc	1015.09	K	Joback Method
tf	476.01	K	Joback Method
vc	0.932	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.35	J/molxK	802.95	Joback Method
cpg	692.76	J/molxK	838.31	Joback Method
cpg	705.16	J/molxK	873.66	Joback Method
cpg	716.58	J/molxK	909.02	Joback Method
cpg	727.04	J/molxK	944.38	Joback Method
cpg	736.58	J/molxK	979.73	Joback Method
cpg	745.21	J/molxK	1015.09	Joback Method
dvisc	0.0007650	Paxs	476.01	Joback Method

dvisc	0.0004264	Paxs	530.50	Joback Method
dvisc	0.0002650	Paxs	584.99	Joback Method
dvisc	0.0001786	Paxs	639.48	Joback Method
dvisc	0.0001281	Paxs	693.97	Joback Method
dvisc	0.0000964	Paxs	748.46	Joback Method
dvisc	0.0000754	Paxs	802.95	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=U405284&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405284&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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