

# Glutaric acid, 3-chlorophenyl 2,6-dimethoxyphenyl ester

<b>Inchi:</b>	InChI=1S/C19H19ClO6/c1-23-15-8-4-9-16(24-2)19(15)26-18(22)11-5-10-17(21)25-14-7-3
<b>InchiKey:</b>	LYRNWKYSYAKKDI-UHFFFAOYSA-N
<b>Formula:</b>	C19H19ClO6
<b>SMILES:</b>	COc1cccc(OC)c1OC(=O)CCCC(=O)Oc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	378.80

## Physical Properties

Property code	Value	Unit	Source
gf	-384.74	kJ/mol	Joback Method
hf	-766.62	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	91.94	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.038		Crippen Method
mcvol	269.910	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2892.00		NIST Webbook
rinpol	2892.00		NIST Webbook
tb	937.27	K	Joback Method
tc	1166.37	K	Joback Method
tf	612.99	K	Joback Method
vc	1.016	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.65	J/molxK	937.27	Joback Method
cpg	807.51	J/molxK	975.45	Joback Method
cpg	816.86	J/molxK	1013.64	Joback Method
cpg	824.68	J/molxK	1051.82	Joback Method
cpg	830.97	J/molxK	1090.00	Joback Method
cpg	835.70	J/molxK	1128.18	Joback Method
cpg	838.88	J/molxK	1166.37	Joback Method
dvisc	0.0001937	Paxs	612.99	Joback Method

dvisc	0.0001275	Paxs	667.04	Joback Method
dvisc	0.0000893	Paxs	721.08	Joback Method
dvisc	0.0000658	Paxs	775.13	Joback Method
dvisc	0.0000504	Paxs	829.18	Joback Method
dvisc	0.0000399	Paxs	883.22	Joback Method
dvisc	0.0000325	Paxs	937.27	Joback Method

## Sources

<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>
<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=U392008&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392008&amp;Units=SI</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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