

# Glutaric acid, di(4-chloro-3-methylphenyl) ester

Inchi:	InChI=1S/C19H18Cl2O4/c1-12-10-14(6-8-16(12)20)24-18(22)4-3-5-19(23)25-15-7-9-17(2)
InchiKey:	YKPQLSLQJGNQBX-UHFFFAOYSA-N
Formula:	C19H18Cl2O4
SMILES:	<chem>Cc1cc(OC(=O)CCCC(=O)Oc2ccc(Cl)c(C)c2)ccc1Cl</chem>
Mol. weight [g/mol]:	381.25

## Physical Properties

Property code	Value	Unit	Source
gf	-196.30	kJ/mol	Joback Method
hf	-529.39	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	92.17	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.292		Crippen Method
mcvol	270.410	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpola	3031.00		NIST Webbook
tb	934.84	K	Joback Method
tc	1169.45	K	Joback Method
tf	610.97	K	Joback Method
vc	1.030	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.29	J/molxK	934.84	Joback Method
cpg	806.69	J/molxK	1130.35	Joback Method
cpg	800.70	J/molxK	1091.25	Joback Method
cpg	793.48	J/molxK	1052.15	Joback Method
cpg	785.03	J/molxK	1013.04	Joback Method
cpg	775.30	J/molxK	973.94	Joback Method
cpg	811.48	J/molxK	1169.45	Joback Method
dvisc	0.0000511	Paxs	934.84	Joback Method
dvisc	0.0000624	Paxs	880.86	Joback Method

dvisc	0.0000782	Paxs	826.88	Joback Method
dvisc	0.0001011	Paxs	772.90	Joback Method
dvisc	0.0001358	Paxs	718.93	Joback Method
dvisc	0.0001914	Paxs	664.95	Joback Method
dvisc	0.0002867	Paxs	610.97	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=U358807&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358807&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>mccvol:</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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