

# Glutaric acid, 2,3-dichlorophenyl 2-methoxyphenyl ester

<b>Inchi:</b>	InChI=1S/C18H16Cl2O5/c1-23-13-7-2-3-8-14(13)24-16(21)10-5-11-17(22)25-15-9-4-6-12
<b>InchiKey:</b>	AZCCQTSLVDPDJRY-UHFFFAOYSA-N
<b>Formula:</b>	C18H16Cl2O5
<b>SMILES:</b>	COc1ccccc1OC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	383.22

## Physical Properties

Property code	Value	Unit	Source
gf	-300.09	kJ/mol	Joback Method
hf	-629.50	kJ/mol	Joback Method
hfus	44.45	kJ/mol	Joback Method
hvap	91.69	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.683		Crippen Method
mcvol	262.190	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	2938.00		NIST Webbook
rinpol	2938.00		NIST Webbook
tb	929.40	K	Joback Method
tc	1163.97	K	Joback Method
tf	609.41	K	Joback Method
vc	0.992	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.42	J/molxK	929.40	Joback Method
cpg	771.95	J/molxK	1124.88	Joback Method
cpg	767.14	J/molxK	1085.78	Joback Method
cpg	760.99	J/molxK	1046.69	Joback Method
cpg	753.49	J/molxK	1007.59	Joback Method
cpg	744.63	J/molxK	968.50	Joback Method
cpg	775.43	J/molxK	1163.97	Joback Method
dvisc	0.0000431	Paxs	929.40	Joback Method

dvisc	0.0000528	Paxs	876.07	Joback Method
dvisc	0.0000666	Paxs	822.74	Joback Method
dvisc	0.0000866	Paxs	769.41	Joback Method
dvisc	0.0001171	Paxs	716.07	Joback Method
dvisc	0.0001662	Paxs	662.74	Joback Method
dvisc	0.0002510	Paxs	609.41	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U391766&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391766&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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