

# Glutaric acid, 2,3-dichlorophenyl 4-cyanophenyl ester

<b>Inchi:</b>	InChI=1S/C18H13Cl2NO4/c19-14-3-1-4-15(18(14)20)25-17(23)6-2-5-16(22)24-13-9-7-12
<b>InchiKey:</b>	HFFRPOYEXYUJQW-UHFFFAOYSA-N
<b>Formula:</b>	C18H13Cl2NO4
<b>SMILES:</b>	N#Cc1ccc(OC(=O)CCCC(=O)Oc2cccc(Cl)c2Cl)cc1
<b>Mol. weight [g/mol]:</b>	378.21

## Physical Properties

Property code	Value	Unit	Source
gf	-61.91	kJ/mol	Joback Method
hf	-332.40	kJ/mol	Joback Method
hfus	44.76	kJ/mol	Joback Method
hvap	99.76	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.546		Crippen Method
mcvol	257.700	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	3105.00		NIST Webbook
rinpol	3105.00		NIST Webbook
tb	1009.06	K	Joback Method
tc	1256.32	K	Joback Method
tf	652.17	K	Joback Method
vc	1.000	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.63	J/molxK	1009.06	Joback Method
cpg	718.93	J/molxK	1050.27	Joback Method
cpg	724.98	J/molxK	1091.48	Joback Method
cpg	729.81	J/molxK	1132.69	Joback Method
cpg	733.44	J/molxK	1173.90	Joback Method
cpg	735.90	J/molxK	1215.11	Joback Method
cpg	737.23	J/molxK	1256.32	Joback Method

# Sources

<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=U393280&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393280&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvp:</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>rlnol:</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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