

# Glutaric acid, 2-chloro-6-fluorophenyl 2-chloro-5-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C18H15Cl2FO4/c1-11-8-9-12(19)15(10-11)24-16(22)6-3-7-17(23)25-18-13(20)
<b>InchiKey:</b>	HVLIVOWAYWXLTC-UHFFFAOYSA-N
<b>Formula:</b>	C18H15Cl2FO4
<b>SMILES:</b>	<chem>Cc1ccc(Cl)c(OC(=O)CCCC(=O)Oc2c(F)cccc2Cl)c1</chem>
<b>Mol. weight [g/mol]:</b>	385.21

## Physical Properties

Property code	Value	Unit	Source
gf	-399.53	kJ/mol	Joback Method
hf	-704.86	kJ/mol	Joback Method
hfus	45.95	kJ/mol	Joback Method
hvap	89.13	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.122		Crippen Method
mvol	258.090	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	2721.00		NIST Webbook
rinpol	2721.00		NIST Webbook
tb	911.23	K	Joback Method
tc	1141.06	K	Joback Method
tf	600.29	K	Joback Method
vc	0.992	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.97	J/molxK	911.23	Joback Method
cpg	725.43	J/molxK	949.54	Joback Method
cpg	734.70	J/molxK	987.84	Joback Method
cpg	742.81	J/molxK	1026.15	Joback Method
cpg	749.76	J/molxK	1064.45	Joback Method
cpg	755.58	J/molxK	1102.76	Joback Method
cpg	760.28	J/molxK	1141.06	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393426&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393426&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>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>rinp:</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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