

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

<b>Inchi:</b>	InChI=1S/C18H16ClFO4/c1-12-9-10-13(19)16(11-12)24-18(22)8-4-7-17(21)23-15-6-3-2-5
<b>InchiKey:</b>	LXQMIVGAGWKLHY-UHFFFAOYSA-N
<b>Formula:</b>	C18H16ClFO4
<b>SMILES:</b>	<chem>Cc1ccc(Cl)c(OC(=O)CCCC(=O)Oc2ccccc2F)c1</chem>
<b>Mol. weight [g/mol]:</b>	350.77

## Physical Properties

Property code	Value	Unit	Source
gf	-377.97	kJ/mol	Joback Method
hf	-677.65	kJ/mol	Joback Method
hfus	42.14	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.469		Crippen Method
mvol	245.850	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	2571.00		NIST Webbook
rinpol	2571.00		NIST Webbook
tb	868.82	K	Joback Method
tc	1094.47	K	Joback Method
tf	557.85	K	Joback Method
vc	0.943	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.81	J/mol×K	868.82	Joback Method
cpg	707.68	J/mol×K	906.43	Joback Method
cpg	718.38	J/mol×K	944.04	Joback Method
cpg	727.92	J/mol×K	981.65	Joback Method
cpg	736.34	J/mol×K	1019.26	Joback Method
cpg	743.66	J/mol×K	1056.87	Joback Method
cpg	749.88	J/mol×K	1094.47	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U393423&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393423&amp;Units=SI</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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