

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

<b>Inchi:</b>	InChI=1S/C17H13ClF2O4/c18-11-5-3-7-13(20)17(11)24-16(22)10-4-9-15(21)23-14-8-2-1
<b>InchiKey:</b>	SDXOJYQPBQFUHK-UHFFFAOYSA-N
<b>Formula:</b>	C17H13ClF2O4
<b>SMILES:</b>	O=C(CCCC(=O)Oc1c(F)ccc1Cl)Oc1ccccc1F
<b>Mol. weight [g/mol]:</b>	354.73

## Physical Properties

Property code	Value	Unit	Source
gf	-581.20	kJ/mol	Joback Method
hf	-853.12	kJ/mol	Joback Method
hfus	42.63	kJ/mol	Joback Method
hvap	81.04	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.300		Crippen Method
mvol	233.530	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	2409.00		NIST Webbook
rinpol	2409.00		NIST Webbook
tb	845.21	K	Joback Method
tc	1065.97	K	Joback Method
tf	547.17	K	Joback Method
vc	0.904	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.75	J/mol×K	845.21	Joback Method
cpg	658.94	J/mol×K	882.00	Joback Method
cpg	669.05	J/mol×K	918.80	Joback Method
cpg	678.11	J/mol×K	955.59	Joback Method
cpg	686.12	J/mol×K	992.38	Joback Method
cpg	693.11	J/mol×K	1029.17	Joback Method
cpg	699.10	J/mol×K	1065.97	Joback Method

# Sources

<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=U391585&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391585&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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