

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

<b>Inchi:</b>	InChI=1S/C16H20ClFO4/c1-3-6-11(2)21-14(19)9-5-10-15(20)22-16-12(17)7-4-8-13(16)1
<b>InchiKey:</b>	VCGXNGNQHVVSJLE-UHFFFAOYSA-N
<b>Formula:</b>	C16H20ClFO4
<b>SMILES:</b>	CCCC(C)OC(=O)CCCC(=O)Oc1c(F)cccc1Cl
<b>Mol. weight [g/mol]:</b>	330.78

## Physical Properties

Property code	Value	Unit	Source
gf	-500.03	kJ/mol	Joback Method
hf	-866.71	kJ/mol	Joback Method
hfus	39.79	kJ/mol	Joback Method
hvap	76.30	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.287		Crippen Method
mvol	241.430	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
tb	790.96	K	Joback Method
tc	993.83	K	Joback Method
tf	481.37	K	Joback Method
vc	0.932	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.35	J/mol×K	790.96	Joback Method
cpg	695.94	J/mol×K	824.77	Joback Method
cpg	708.56	J/mol×K	858.58	Joback Method
cpg	720.22	J/mol×K	892.40	Joback Method
cpg	730.94	J/mol×K	926.21	Joback Method
cpg	740.72	J/mol×K	960.02	Joback Method
cpg	749.58	J/mol×K	993.83	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=U391430&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391430&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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