

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

<b>Inchi:</b>	InChI=1S/C17H22ClFO4/c1-3-6-12(2)11-22-15(20)9-5-10-16(21)23-17-13(18)7-4-8-14(1)
<b>InchiKey:</b>	HGACFZAHIGBIAO-UHFFFAOYSA-N
<b>Formula:</b>	C17H22ClFO4
<b>SMILES:</b>	CCCC(C)COC(=O)CCCC(=O)Oc1c(F)cccc1Cl
<b>Mol. weight [g/mol]:</b>	344.81

## Physical Properties

Property code	Value	Unit	Source
gf	-491.61	kJ/mol	Joback Method
hf	-887.35	kJ/mol	Joback Method
hfus	42.38	kJ/mol	Joback Method
hvap	78.53	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.534		Crippen Method
mvol	255.520	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	813.84	K	Joback Method
tc	1016.05	K	Joback Method
tf	492.64	K	Joback Method
vc	0.989	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.44	J/mol×K	813.84	Joback Method
cpg	752.32	J/mol×K	847.54	Joback Method
cpg	765.19	J/mol×K	881.24	Joback Method
cpg	777.06	J/mol×K	914.95	Joback Method
cpg	787.95	J/mol×K	948.65	Joback Method
cpg	797.87	J/mol×K	982.35	Joback Method
cpg	806.84	J/mol×K	1016.05	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=U391711&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391711&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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