

# Glutaric acid, 2-chloro-6-fluorophenyl 2,3,5-trichlorophenyl ester

**Inchi:** InChI=1S/C17H11Cl4FO4/c18-9-7-11(20)16(21)13(8-9)25-14(23)5-2-6-15(24)26-17-10(1)  
**InchiKey:** HXMPVBZBIXERDE-UHFFFAOYSA-N  
**Formula:** C17H11Cl4FO4  
**SMILES:** O=C(CCCC(=O)Oc1c(F)cccc1Cl)Oc1cc(Cl)cc(Cl)c1Cl  
**Mol. weight [g/mol]:** 440.08

## Physical Properties

Property code	Value	Unit	Source
gf	-441.44	kJ/mol	Joback Method
hf	-727.17	kJ/mol	Joback Method
hfus	51.37	kJ/mol	Joback Method
hvap	96.33	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	6.121		Crippen Method
mvol	268.480	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	2943.00		NIST Webbook
rinpol	2943.00		NIST Webbook
tb	968.19	K	Joback Method
tc	1207.34	K	Joback Method
tf	661.38	K	Joback Method
vc	1.034	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.18	J/molxK	968.19	Joback Method
cpg	700.75	J/molxK	1008.05	Joback Method
cpg	707.14	J/molxK	1047.91	Joback Method
cpg	712.36	J/molxK	1087.76	Joback Method
cpg	716.42	J/molxK	1127.62	Joback Method
cpg	719.34	J/molxK	1167.48	Joback Method
cpg	721.13	J/molxK	1207.34	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=U392184&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392184&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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