

# Succinic acid, 2-chloro-6-fluorophenyl 2-methoxyphenyl ester

**Inchi:** InChI=1S/C17H14ClFO5/c1-22-13-7-2-3-8-14(13)23-15(20)9-10-16(21)24-17-11(18)5-4-  
**InchiKey:** LWGRHNRPRDVPIV-UHFFFAOYSA-N  
**Formula:** C17H14ClFO5  
**SMILES:** COc1ccccc1OC(=O)CCC(=O)Oc1c(F)cccc1Cl  
**Mol. weight [g/mol]:** 352.74

## Physical Properties

Property code	Value	Unit	Source
gf	-491.39	kJ/mol	Joback Method
hf	-789.23	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	84.26	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.779		Crippen Method
mvol	237.630	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	2537.00		NIST Webbook
rinpol	2537.00		NIST Webbook
tb	868.36	K	Joback Method
tc	1094.78	K	Joback Method
tf	568.81	K	Joback Method
vc	0.904	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.73	J/mol×K	868.36	Joback Method
cpg	676.82	J/mol×K	906.10	Joback Method
cpg	686.68	J/mol×K	943.83	Joback Method
cpg	695.31	J/mol×K	981.57	Joback Method
cpg	702.72	J/mol×K	1019.31	Joback Method
cpg	708.90	J/mol×K	1057.04	Joback Method
cpg	713.86	J/mol×K	1094.78	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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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=U389712&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389712&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>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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