

# Succinic acid, 2-chloro-6-fluorophenyl 3-methylbut-3-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C15H16ClFO4/c1-10(2)8-9-20-13(18)6-7-14(19)21-15-11(16)4-3-5-12(15)17/h
<b>InchiKey:</b>	UAGNIXAPXGYMHG-UHFFFAOYSA-N
<b>Formula:</b>	C15H16ClFO4
<b>SMILES:</b>	<chem>C=C(C)CCOC(=O)CCC(=O)Oc1c(F)cccc1Cl</chem>
<b>Mol. weight [g/mol]:</b>	314.74

## Physical Properties

Property code	Value	Unit	Source
gf	-426.72	kJ/mol	Joback Method
hf	-725.15	kJ/mol	Joback Method
hfus	38.13	kJ/mol	Joback Method
hvap	73.87	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.674		Crippen Method
mcvol	223.040	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	765.08	K	Joback Method
tc	971.49	K	Joback Method
tf	469.38	K	Joback Method
vc	0.865	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.07	J/molxK	765.08	Joback Method
cpg	613.72	J/molxK	799.48	Joback Method
cpg	625.48	J/molxK	833.88	Joback Method
cpg	636.36	J/molxK	868.29	Joback Method
cpg	646.39	J/molxK	902.69	Joback Method
cpg	655.56	J/molxK	937.09	Joback Method
cpg	663.90	J/molxK	971.49	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=U391139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391139&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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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