

# Succinic acid, 2-chloro-6-fluorophenyl cis-hex-2-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C16H18ClFO4/c1-2-3-4-5-11-21-14(19)9-10-15(20)22-16-12(17)7-6-8-13(16)1
<b>InchiKey:</b>	QKCWGWZFEICSPV-PLNGDYQASA-N
<b>Formula:</b>	C16H18ClFO4
<b>SMILES:</b>	CCCC=CCOC(=O)CCC(=O)Oc1c(F)cccc1Cl
<b>Mol. weight [g/mol]:</b>	328.76

## Physical Properties

Property code	Value	Unit	Source
gf	-417.37	kJ/mol	Joback Method
hf	-744.21	kJ/mol	Joback Method
hfus	43.51	kJ/mol	Joback Method
hvap	76.65	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.064		Crippen Method
mvol	237.130	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2206.00		NIST Webbook
rinpol	2206.00		NIST Webbook
tb	795.56	K	Joback Method
tc	1001.35	K	Joback Method
tf	491.29	K	Joback Method
vc	0.918	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.06	J/molxK	795.56	Joback Method
cpg	668.95	J/molxK	829.86	Joback Method
cpg	680.93	J/molxK	864.16	Joback Method
cpg	692.04	J/molxK	898.46	Joback Method
cpg	702.29	J/molxK	932.75	Joback Method
cpg	711.70	J/molxK	967.05	Joback Method
cpg	720.30	J/molxK	1001.35	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U391304&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391304&amp;Units=SI</a>
<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>

# 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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