

# Succinic acid, ethyl 1-(2-fluorophenyl)ethyl ester

Inchi:	InChI=1S/C14H17FO4/c1-3-18-13(16)8-9-14(17)19-10(2)11-6-4-5-7-12(11)15/h4-7,10H,3
InchiKey:	CWWHIVFYWBWDDF-UHFFFAOYSA-N
Formula:	C14H17FO4
SMILES:	CCOC(=O)CCC(=O)OC(C)c1ccccc1F
Mol. weight [g/mol]:	268.28

## Physical Properties

Property code	Value	Unit	Source
gf	-495.31	kJ/mol	Joback Method
hf	-798.22	kJ/mol	Joback Method
hfus	30.80	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.773		Crippen Method
mcvol	201.010	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook
tb	702.79	K	Joback Method
tc	904.30	K	Joback Method
tf	416.39	K	Joback Method
vc	0.771	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.41	J/mol×K	702.79	Joback Method
cpg	562.43	J/mol×K	736.37	Joback Method
cpg	575.58	J/mol×K	769.96	Joback Method
cpg	587.86	J/mol×K	803.54	Joback Method
cpg	599.28	J/mol×K	837.13	Joback Method
cpg	609.84	J/mol×K	870.71	Joback Method
cpg	619.56	J/mol×K	904.30	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=U381390&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381390&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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