

# Succinic acid, but-3-yn-2-yl 2-fluorophenyl ester

Inchi:	InChI=1S/C14H13FO4/c1-3-10(2)18-13(16)8-9-14(17)19-12-7-5-4-6-11(12)15/h1,4-7,10H
InchiKey:	BWKSUGJINUWRLR-UHFFFAOYSA-N
Formula:	C14H13FO4
SMILES:	C#CC(C)OC(=O)CCC(=O)Oc1ccccc1F
Mol. weight [g/mol]:	264.25

## Physical Properties

Property code	Value	Unit	Source
gf	-272.24	kJ/mol	Joback Method
hf	-506.32	kJ/mol	Joback Method
hfus	33.77	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.076		Crippen Method
mcvol	192.410	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1748.00		NIST Webbook
rinpol	1748.00		NIST Webbook
tb	692.91	K	Joback Method
tc	905.65	K	Joback Method
tf	463.36	K	Joback Method
vc	0.734	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.89	J/mol×K	692.91	Joback Method
cpg	513.81	J/mol×K	728.37	Joback Method
cpg	525.85	J/mol×K	763.82	Joback Method
cpg	537.05	J/mol×K	799.28	Joback Method
cpg	547.40	J/mol×K	834.74	Joback Method
cpg	556.93	J/mol×K	870.19	Joback Method
cpg	565.65	J/mol×K	905.65	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U390304&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390304&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>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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