

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

<b>Inchi:</b>	InChI=1S/C14H13ClO4/c1-3-10(2)18-13(16)8-9-14(17)19-12-7-5-4-6-11(12)15/h1,4-7,10
<b>InchiKey:</b>	BCMMGLNMLSSRTN-UHFFFAOYSA-N
<b>Formula:</b>	C14H13ClO4
<b>SMILES:</b>	C#CC(C)OC(=O)CCC(=O)Oc1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	280.70

## Physical Properties

Property code	Value	Unit	Source
gf	-89.36	kJ/mol	Joback Method
hf	-325.95	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	71.86	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.590		Crippen Method
mcvol	202.880	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	731.07	K	Joback Method
tc	955.87	K	Joback Method
tf	492.69	K	Joback Method
vc	0.764	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.09	J/mol×K	731.07	Joback Method
cpg	529.53	J/mol×K	768.54	Joback Method
cpg	541.03	J/mol×K	806.00	Joback Method
cpg	551.60	J/mol×K	843.47	Joback Method
cpg	561.28	J/mol×K	880.94	Joback Method
cpg	570.06	J/mol×K	918.40	Joback Method
cpg	577.97	J/mol×K	955.87	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U389795&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389795&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>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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