

# Succinic acid, but-3-yn-2-yl cis-pent-2-en-1-yl ester

Inchi:	InChI=1S/C13H18O4/c1-4-6-7-10-16-12(14)8-9-13(15)17-11(3)5-2/h2,6-7,11H,4,8-10H2,
InchiKey:	XMRSYNBCSDHMEZ-SREVYHEPSA-N
Formula:	C13H18O4
SMILES:	C#CC(C)OC(=O)CCC(=O)OCC=CCC
Mol. weight [g/mol]:	238.28

## Physical Properties

Property code	Value	Unit	Source
gf	-108.41	kJ/mol	Joback Method
hf	-397.41	kJ/mol	Joback Method
hfus	34.65	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	1.841		Crippen Method
mcvol	196.010	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1591.00		NIST Webbook
rinpol	1591.00		NIST Webbook
tb	643.26	K	Joback Method
tc	838.20	K	Joback Method
tf	407.48	K	Joback Method
vc	0.748	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.36	J/mol×K	643.26	Joback Method
cpg	516.19	J/mol×K	675.75	Joback Method
cpg	529.29	J/mol×K	708.24	Joback Method
cpg	541.69	J/mol×K	740.73	Joback Method
cpg	553.40	J/mol×K	773.22	Joback Method
cpg	564.44	J/mol×K	805.71	Joback Method
cpg	574.82	J/mol×K	838.20	Joback Method

# Sources

<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=U391256&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391256&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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