

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

Inchi:	InChI=1S/C11H16O5/c1-4-9(2)16-11(13)6-5-10(12)15-8-7-14-3/h1,9H,5-8H2,2-3H3
InchiKey:	KIYNCDUGEZAJOH-UHFFFAOYSA-N
Formula:	C11H16O5
SMILES:	C#CC(C)OC(=O)CCC(=O)OCCOC
Mol. weight [g/mol]:	228.24

## Physical Properties

Property code	Value	Unit	Source
gf	-310.47	kJ/mol	Joback Method
hf	-605.57	kJ/mol	Joback Method
hfus	30.46	kJ/mol	Joback Method
hvap	60.27	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.521		Crippen Method
mvol	178.000	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
tb	615.76	K	Joback Method
tc	806.65	K	Joback Method
tf	412.25	K	Joback Method
vc	0.673	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.04	J/molxK	615.76	Joback Method
cpg	461.92	J/molxK	647.58	Joback Method
cpg	474.20	J/molxK	679.39	Joback Method
cpg	485.89	J/molxK	711.21	Joback Method
cpg	496.97	J/molxK	743.02	Joback Method
cpg	507.44	J/molxK	774.84	Joback Method
cpg	517.29	J/molxK	806.65	Joback Method

# Sources

<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=U390733&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390733&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>h vap:</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>r in pol:</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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