

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

Inchi:	InChI=1S/C13H20O4/c1-6-10(4)16-12(14)7-8-13(15)17-11(5)9(2)3/h1,9-11H,7-8H2,2-5H
InchiKey:	JEWISMGVIZJBAG-UHFFFAOYSA-N
Formula:	C13H20O4
SMILES:	C#CC(C)OC(=O)CCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	240.30

## Physical Properties

Property code	Value	Unit	Source
gf	-193.51	kJ/mol	Joback Method
hf	-525.19	kJ/mol	Joback Method
hfus	27.41	kJ/mol	Joback Method
hvap	61.54	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	1.919		Crippen Method
mvol	200.310	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	638.22	K	Joback Method
tc	832.89	K	Joback Method
tf	382.56	K	Joback Method
vc	0.755	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.70	J/molxK	638.22	Joback Method
cpg	539.63	J/molxK	670.67	Joback Method
cpg	553.79	J/molxK	703.11	Joback Method
cpg	567.20	J/molxK	735.56	Joback Method
cpg	579.85	J/molxK	768.00	Joback Method
cpg	591.75	J/molxK	800.45	Joback Method
cpg	602.92	J/molxK	832.89	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=U390580&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390580&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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