

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

Inchi:	InChI=1S/C14H20O4/c1-4-6-7-8-11-17-13(15)9-10-14(16)18-12(3)5-2/h2,7-8,12H,4,6,9-11
InchiKey:	XKPSVFSAJQUZQW-FPLPWBNLSA-N
Formula:	C14H20O4
SMILES:	<chem>C#CC(C)OC(=O)CCC(=O)OCC=CCCC</chem>
Mol. weight [g/mol]:	252.31

## Physical Properties

Property code	Value	Unit	Source
gf	-99.99	kJ/mol	Joback Method
hf	-418.05	kJ/mol	Joback Method
hfus	37.24	kJ/mol	Joback Method
hvap	64.50	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.231		Crippen Method
mvol	210.100	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	666.14	K	Joback Method
tc	859.01	K	Joback Method
tf	418.75	K	Joback Method
vc	0.803	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.93	J/mol×K	666.14	Joback Method
cpg	568.31	J/mol×K	698.28	Joback Method
cpg	581.93	J/mol×K	730.43	Joback Method
cpg	594.82	J/mol×K	762.57	Joback Method
cpg	606.99	J/mol×K	794.72	Joback Method
cpg	618.45	J/mol×K	826.86	Joback Method
cpg	629.23	J/mol×K	859.01	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=U391296&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391296&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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