

# Succinic acid, hex-4-yn-3-yl but-3-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C14H20O4/c1-4-7-11-17-13(15)9-10-14(16)18-12(6-3)8-5-2/h4,12H,1,6-7,9-11
<b>InchiKey:</b>	DQKSRAISZVQSHQ-UHFFFAOYSA-N
<b>Formula:</b>	C14H20O4
<b>SMILES:</b>	<chem>C=CCCOC(=O)CCC(=O)OC(C#CC)CC</chem>
<b>Mol. weight [g/mol]:</b>	252.31

## Physical Properties

Property code	Value	Unit	Source
gf	-112.64	kJ/mol	Joback Method
hf	-429.44	kJ/mol	Joback Method
hfus	35.91	kJ/mol	Joback Method
hvap	66.16	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.231		Crippen Method
mvol	210.100	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	1723.00		NIST Webbook
rinpol	1723.00		NIST Webbook
tb	677.54	K	Joback Method
tc	874.77	K	Joback Method
tf	481.20	K	Joback Method
vc	0.804	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.91	J/molxK	677.54	Joback Method
cpg	570.67	J/molxK	710.41	Joback Method
cpg	584.66	J/molxK	743.28	Joback Method
cpg	597.87	J/molxK	776.16	Joback Method
cpg	610.31	J/molxK	809.03	Joback Method
cpg	621.98	J/molxK	841.90	Joback Method
cpg	632.89	J/molxK	874.77	Joback Method

# Sources

<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=U391191&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391191&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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