

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

<b>Inchi:</b>	InChI=1S/C14H22O4/c1-5-8-12(7-3)18-14(16)10-9-13(15)17-11(4)6-2/h2,11-12H,5,7-10H
<b>InchiKey:</b>	MKEUJAFRCRSUKY-UHFFFAOYSA-N
<b>Formula:</b>	C14H22O4
<b>SMILES:</b>	C#CC(C)OC(=O)CCC(=O)OC(CC)CCC
<b>Mol. weight [g/mol]:</b>	254.32

## Physical Properties

Property code	Value	Unit	Source
gf	-182.65	kJ/mol	Joback Method
hf	-540.55	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.453		Crippen Method
mvol	214.400	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
tb	661.54	K	Joback Method
tc	851.00	K	Joback Method
tf	408.83	K	Joback Method
vc	0.818	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.39	J/mol×K	661.54	Joback Method
cpg	591.56	J/mol×K	693.12	Joback Method
cpg	605.95	J/mol×K	724.69	Joback Method
cpg	619.58	J/mol×K	756.27	Joback Method
cpg	632.46	J/mol×K	787.85	Joback Method
cpg	644.59	J/mol×K	819.43	Joback Method
cpg	655.98	J/mol×K	851.00	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=U390545&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390545&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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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