

# Succinic acid, 3-methylbut-2-yl non-5-yn-3-yl ester

Inchi:	InChI=1S/C18H30O4/c1-6-8-9-10-11-16(7-2)22-18(20)13-12-17(19)21-15(5)14(3)4/h14-1
InchiKey:	DBVNUKRTGQHKMA-UHFFFAOYSA-N
Formula:	C18H30O4
SMILES:	CCCC#CCC(CC)OC(=O)CCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	310.43

## Physical Properties

Property code	Value	Unit	Source
gf	-171.68	kJ/mol	Joback Method
hf	-647.99	kJ/mol	Joback Method
hfus	40.50	kJ/mol	Joback Method
hvap	74.96	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.870		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
tb	771.50	K	Joback Method
tc	966.35	K	Joback Method
tf	498.04	K	Joback Method
vc	1.036	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.50	J/mol×K	771.50	Joback Method
cpg	820.75	J/mol×K	803.98	Joback Method
cpg	836.98	J/mol×K	836.45	Joback Method
cpg	852.19	J/mol×K	868.93	Joback Method
cpg	866.40	J/mol×K	901.40	Joback Method
cpg	879.61	J/mol×K	933.88	Joback Method
cpg	891.84	J/mol×K	966.35	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=U391008&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391008&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>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>rlnol:</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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