

# Succinic acid, but-3-yn-2-yl cis-4-methylcyclohexyl ester

<b>Inchi:</b>	InChI=1S/C15H22O4/c1-4-12(3)18-14(16)9-10-15(17)19-13-7-5-11(2)6-8-13/h1,11-13H,5
<b>InchiKey:</b>	GVMREGMLJWCQHZ-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O4
<b>SMILES:</b>	C#CC(C)OC(=O)CCC(=O)OC1CCC(C)CC1
<b>Mol. weight [g/mol]:</b>	266.33

## Physical Properties

Property code	Value	Unit	Source
gf	-155.05	kJ/mol	Joback Method
hf	-521.93	kJ/mol	Joback Method
hfus	32.54	kJ/mol	Joback Method
hvap	66.89	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.453		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	699.74	K	Joback Method
tc	911.37	K	Joback Method
tf	438.24	K	Joback Method
vc	0.811	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.25	J/mol×K	699.74	Joback Method
cpg	643.39	J/mol×K	735.01	Joback Method
cpg	660.35	J/mol×K	770.28	Joback Method
cpg	676.15	J/mol×K	805.56	Joback Method
cpg	690.79	J/mol×K	840.83	Joback Method
cpg	704.30	J/mol×K	876.10	Joback Method
cpg	716.67	J/mol×K	911.37	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=U390055&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390055&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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