

# Succinic acid, tridec-2-yn-1-yl 2-hexyl ester

**Inchi:** InChI=1S/C23H40O4/c1-4-6-8-9-10-11-12-13-14-15-16-20-26-22(24)18-19-23(25)27-21(  
**InchiKey:** GTRBLZGGLNPXLX-UHFFFAOYSA-N  
**Formula:** C23H40O4  
**SMILES:** CCCCCCCCCC#CCOC(=O)CCC(=O)OC(C)CCCC  
**Mol. weight [g/mol]:** 380.56

## Physical Properties

Property code	Value	Unit	Source
gf	-124.70	kJ/mol	Joback Method
hf	-740.63	kJ/mol	Joback Method
hfus	60.50	kJ/mol	Joback Method
hvap	86.87	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	5.966		Crippen Method
mvol	341.210	ml/mol	McGowan Method
pc	997.65	kPa	Joback Method
rinpol	2624.00		NIST Webbook
rinpol	2624.00		NIST Webbook
tb	886.78	K	Joback Method
tc	1086.62	K	Joback Method
tf	584.39	K	Joback Method
vc	1.327	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.99	J/mol×K	886.78	Joback Method
cpg	1121.36	J/mol×K	920.09	Joback Method
cpg	1138.48	J/mol×K	953.39	Joback Method
cpg	1154.37	J/mol×K	986.70	Joback Method
cpg	1169.05	J/mol×K	1020.00	Joback Method
cpg	1182.55	J/mol×K	1053.31	Joback Method
cpg	1194.89	J/mol×K	1086.62	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U390696&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390696&amp;Units=SI</a>
<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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>

# 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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