

# Succinic acid, tridec-2-yn-1-yl 4-heptyl ester

**Inchi:** InChI=1S/C24H42O4/c1-4-7-8-9-10-11-12-13-14-15-16-21-27-23(25)19-20-24(26)28-22(29)  
**InchiKey:** LUNABNIPHZYRDK-UHFFFAOYSA-N  
**Formula:** C24H42O4  
**SMILES:** CCCCCCCCCC#CCOC(=O)CCC(=O)OC(CCC)CCC  
**Mol. weight [g/mol]:** 394.59

## Physical Properties

Property code	Value	Unit	Source
gf	-116.28	kJ/mol	Joback Method
hf	-761.27	kJ/mol	Joback Method
hfus	63.09	kJ/mol	Joback Method
hvap	89.09	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.356		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	939.79	kPa	Joback Method
rinpol	2662.00		NIST Webbook
rinpol	2662.00		NIST Webbook
tb	909.66	K	Joback Method
tc	1113.76	K	Joback Method
tf	595.66	K	Joback Method
vc	1.383	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.20	J/mol×K	909.66	Joback Method
cpg	1183.91	J/mol×K	943.68	Joback Method
cpg	1201.29	J/mol×K	977.69	Joback Method
cpg	1217.35	J/mol×K	1011.71	Joback Method
cpg	1232.13	J/mol×K	1045.73	Joback Method
cpg	1245.66	J/mol×K	1079.74	Joback Method
cpg	1257.97	J/mol×K	1113.76	Joback Method

# Sources

<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.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>
<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=U390484&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390484&amp;Units=SI</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>h vap:</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>r in pol:</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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