

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

<b>Inchi:</b>	InChI=1S/C24H40O4/c1-3-4-5-6-7-8-9-10-11-12-13-20-27-23(25)18-19-24(26)28-22-16-
<b>InchiKey:</b>	NSRULGOTUPNZFY-UHFFFAOYSA-N
<b>Formula:</b>	C24H40O4
<b>SMILES:</b>	CCCCCCCCCCC#CCOC(=O)CCC(=O)OC1CCC(C)CC1
<b>Mol. weight [g/mol]:</b>	392.57

## Physical Properties

Property code	Value	Unit	Source
gf	-97.10	kJ/mol	Joback Method
hf	-722.01	kJ/mol	Joback Method
hfus	59.52	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.966		Crippen Method
mvol	344.440	ml/mol	McGowan Method
pc	1041.93	kPa	Joback Method
rinpol	2842.00		NIST Webbook
rinpol	2842.00		NIST Webbook
tb	924.98	K	Joback Method
tc	1135.84	K	Joback Method
tf	613.80	K	Joback Method
vc	1.321	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.27	J/mol×K	924.98	Joback Method
cpg	1183.93	J/mol×K	960.12	Joback Method
cpg	1200.99	J/mol×K	995.27	Joback Method
cpg	1216.47	J/mol×K	1030.41	Joback Method
cpg	1230.41	J/mol×K	1065.55	Joback Method
cpg	1242.84	J/mol×K	1100.70	Joback Method
cpg	1253.78	J/mol×K	1135.84	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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U390074&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390074&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>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

Latest version available from:

<https://www.chemeo.com/cid/95-679-4/Succinic-acid-tridec-2-yn-1-yl-trans-4-methylcyclohexyl-ester.pdf>

Generated by Cheméo on 2024-04-24 20:29:09.34429145 +0000 UTC m=+16279798.264868761.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.