

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

Inchi:	InChI=1S/C24H33ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-19-28-23(26)17-18-24(27)29-20-21
InchiKey:	MRBOGLKHPVLMEX-UHFFFAOYSA-N
Formula:	C24H33ClO4
SMILES:	CCCCCCCCC#CCOC(=O)CCC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	420.97

## Physical Properties

Property code	Value	Unit	Source
gf	-22.99	kJ/mol	Joback Method
hf	-546.67	kJ/mol	Joback Method
hfus	64.46	kJ/mol	Joback Method
hvap	96.80	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.241		Crippen Method
mvol	343.780	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	3168.00		NIST Webbook
rinpol	3168.00		NIST Webbook
tb	979.19	K	Joback Method
tc	1200.84	K	Joback Method
tf	679.52	K	Joback Method
vc	1.331	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.66	J/molxK	979.19	Joback Method
cpg	1104.39	J/molxK	1016.13	Joback Method
cpg	1117.75	J/molxK	1053.07	Joback Method
cpg	1129.78	J/molxK	1090.01	Joback Method
cpg	1140.52	J/molxK	1126.96	Joback Method
cpg	1150.01	J/molxK	1163.90	Joback Method
cpg	1158.29	J/molxK	1200.84	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=U389685&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389685&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>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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