

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

Inchi:	InChI=1S/C23H31ClO4/c1-2-3-4-5-6-7-8-9-10-11-14-19-27-22(25)17-18-23(26)28-21-16
InchiKey:	UCYMOQZMVCFZSW-UHFFFAOYSA-N
Formula:	C23H31ClO4
SMILES:	CCCCCCCCC#CCOC(=O)CCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	406.94

## Physical Properties

Property code	Value	Unit	Source
gf	-31.41	kJ/mol	Joback Method
hf	-526.03	kJ/mol	Joback Method
hfus	61.87	kJ/mol	Joback Method
hvap	94.58	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.103		Crippen Method
mvol	329.690	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	3012.00		NIST Webbook
rinpol	3012.00		NIST Webbook
tb	956.31	K	Joback Method
tc	1175.32	K	Joback Method
tf	668.25	K	Joback Method
vc	1.274	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.24	J/molxK	956.31	Joback Method
cpg	1043.83	J/molxK	992.81	Joback Method
cpg	1057.10	J/molxK	1029.31	Joback Method
cpg	1069.09	J/molxK	1065.82	Joback Method
cpg	1079.85	J/molxK	1102.32	Joback Method
cpg	1089.40	J/molxK	1138.82	Joback Method
cpg	1097.78	J/molxK	1175.32	Joback Method

# Sources

<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=U389806&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389806&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>

# 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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