

# Succinic acid, 3-chlorophenyl trans-hex-3-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C16H19ClO4/c1-2-3-4-5-11-20-15(18)9-10-16(19)21-14-8-6-7-13(17)12-14/h3-
<b>InchiKey:</b>	SQRAYFATJYUVQL-ONEGZZNKSA-N
<b>Formula:</b>	C16H19ClO4
<b>SMILES:</b>	CCC=CCCOC(=O)CCC(=O)Oc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	310.77

## Physical Properties

Property code	Value	Unit	Source
gf	-212.93	kJ/mol	Joback Method
hf	-536.63	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.925		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
tb	791.31	K	Joback Method
tc	1002.86	K	Joback Method
tf	478.18	K	Joback Method
vc	0.900	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.61	J/molxK	791.31	Joback Method
cpg	663.09	J/molxK	826.57	Joback Method
cpg	675.61	J/molxK	861.83	Joback Method
cpg	687.19	J/molxK	897.09	Joback Method
cpg	697.88	J/molxK	932.35	Joback Method
cpg	707.68	J/molxK	967.60	Joback Method
cpg	716.64	J/molxK	1002.86	Joback Method
dvisc	0.0006625	Paxs	478.18	Joback Method

dvisc	0.0003814	Paxs	530.37	Joback Method
dvisc	0.0002424	Paxs	582.56	Joback Method
dvisc	0.0001660	Paxs	634.75	Joback Method
dvisc	0.0001204	Paxs	686.93	Joback Method
dvisc	0.0000914	Paxs	739.12	Joback Method
dvisc	0.0000719	Paxs	791.31	Joback Method

## Sources

<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=U391119&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391119&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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