

# Succinic acid, 3-chlorophenyl 4-methylpent-2-yl ester

<b>Inchi:</b>	InChI=1S/C16H21ClO4/c1-11(2)9-12(3)20-15(18)7-8-16(19)21-14-6-4-5-13(17)10-14/h4-
<b>InchiKey:</b>	HMUVKWIFXJMIBT-UHFFFAOYSA-N
<b>Formula:</b>	C16H21ClO4
<b>SMILES:</b>	CC(C)CC(C)OC(=O)CCC(=O)Oc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	312.79

## Physical Properties

Property code	Value	Unit	Source
gf	-298.03	kJ/mol	Joback Method
hf	-664.41	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	76.07	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.003		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook
tb	786.27	K	Joback Method
tc	997.58	K	Joback Method
tf	453.26	K	Joback Method
vc	0.908	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.33	J/molxK	786.27	Joback Method
cpg	690.72	J/molxK	821.49	Joback Method
cpg	704.05	J/molxK	856.71	Joback Method
cpg	716.33	J/molxK	891.92	Joback Method
cpg	727.57	J/molxK	927.14	Joback Method
cpg	737.79	J/molxK	962.36	Joback Method
cpg	747.01	J/molxK	997.58	Joback Method
dvisc	0.0009423	Paxs	453.26	Joback Method

dvisc	0.0004823	Paxs	508.76	Joback Method
dvisc	0.0002816	Paxs	564.26	Joback Method
dvisc	0.0001811	Paxs	619.76	Joback Method
dvisc	0.0001252	Paxs	675.27	Joback Method
dvisc	0.0000916	Paxs	730.77	Joback Method
dvisc	0.0000700	Paxs	786.27	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=U390432&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390432&amp;Units=SI</a>

## Legend

<b>cpg:</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>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>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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