

# Succinic acid, 4-chloro-3-methylphenyl 3-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C16H21ClO4/c1-11(2)8-9-20-15(18)6-7-16(19)21-13-4-5-14(17)12(3)10-13/h4-
<b>InchiKey:</b>	FHXJHEYNPXVFJH-UHFFFAOYSA-N
<b>Formula:</b>	C16H21ClO4
<b>SMILES:</b>	<chem>Cc1cc(OC(=O)CCC(=O)OCCC(C)C)ccc1Cl</chem>
<b>Mol. weight [g/mol]:</b>	312.79

## Physical Properties

Property code	Value	Unit	Source
gf	-305.22	kJ/mol	Joback Method
hf	-670.60	kJ/mol	Joback Method
hfus	36.71	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.923		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinsol	2174.00		NIST Webbook
tb	791.69	K	Joback Method
tc	1000.85	K	Joback Method
tf	480.78	K	Joback Method
vc	0.914	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.74	J/molxK	791.69	Joback Method
cpg	735.14	J/molxK	965.99	Joback Method
cpg	725.06	J/molxK	931.13	Joback Method
cpg	713.99	J/molxK	896.27	Joback Method
cpg	701.92	J/molxK	861.41	Joback Method
cpg	688.84	J/molxK	826.55	Joback Method
cpg	744.24	J/molxK	1000.85	Joback Method
dvisc	0.0000767	Paxs	791.69	Joback Method
dvisc	0.0000973	Paxs	739.87	Joback Method

dvisc	0.0001280	Paxs	688.05	Joback Method
dvisc	0.0001760	Paxs	636.24	Joback Method
dvisc	0.0002562	Paxs	584.42	Joback Method
dvisc	0.0004012	Paxs	532.60	Joback Method
dvisc	0.0006920	Paxs	480.78	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=U370967&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370967&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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