

# Succinic acid, 2,4,6-trichlorophenyl 3-methylpentyl ester

<b>Inchi:</b>	InChI=1S/C16H19Cl3O4/c1-3-10(2)6-7-22-14(20)4-5-15(21)23-16-12(18)8-11(17)9-13(16)
<b>InchiKey:</b>	OKKVRDBVMKDKEV-UHFFFAOYSA-N
<b>Formula:</b>	C16H19Cl3O4
<b>SMILES:</b>	CCC(C)CCOC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	381.68

## Physical Properties

Property code	Value	Unit	Source
gf	-338.71	kJ/mol	Joback Method
hf	-713.55	kJ/mol	Joback Method
hfus	44.71	kJ/mol	Joback Method
hvap	86.55	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.312		Crippen Method
mvol	264.140	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2473.00		NIST Webbook
rinpol	2473.00		NIST Webbook
tb	871.53	K	Joback Method
tc	1089.08	K	Joback Method
tf	553.14	K	Joback Method
vc	1.012	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.95	J/molxK	871.53	Joback Method
cpg	732.62	J/molxK	907.79	Joback Method
cpg	743.22	J/molxK	944.05	Joback Method
cpg	752.77	J/molxK	980.31	Joback Method
cpg	761.28	J/molxK	1016.56	Joback Method
cpg	768.76	J/molxK	1052.82	Joback Method
cpg	775.20	J/molxK	1089.08	Joback Method
dvisc	0.0004193	Paxs	553.14	Joback Method

dvisc	0.0002614	Paxs	606.20	Joback Method
dvisc	0.0001759	Paxs	659.27	Joback Method
dvisc	0.0001255	Paxs	712.34	Joback Method
dvisc	0.0000939	Paxs	765.40	Joback Method
dvisc	0.0000729	Paxs	818.46	Joback Method
dvisc	0.0000584	Paxs	871.53	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=U390655&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390655&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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