

# Succinic acid, 2,2-dichloroethyl 4-chloro-2-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C13H13Cl3O4/c1-8-6-9(14)2-3-10(8)20-13(18)5-4-12(17)19-7-11(15)16/h2-3,6
<b>InchiKey:</b>	WSDWWQBQBIXNY-UHFFFAOYSA-N
<b>Formula:</b>	C13H13Cl3O4
<b>SMILES:</b>	Cc1cc(Cl)ccc1OC(=O)CCC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	339.60

## Physical Properties

Property code	Value	Unit	Source
gf	-354.34	kJ/mol	Joback Method
hf	-640.16	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	79.21	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.681		Crippen Method
mvol	221.870	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	797.91	K	Joback Method
tc	1020.41	K	Joback Method
tf	506.81	K	Joback Method
vc	0.845	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.19	J/molxK	797.91	Joback Method
cpg	602.90	J/molxK	983.33	Joback Method
cpg	595.81	J/molxK	946.24	Joback Method
cpg	587.80	J/molxK	909.16	Joback Method
cpg	578.86	J/molxK	872.08	Joback Method
cpg	568.99	J/molxK	834.99	Joback Method
cpg	609.08	J/molxK	1020.41	Joback Method
dvisc	0.0000882	Paxs	797.91	Joback Method

dvisc	0.0001103	Paxs	749.39	Joback Method
dvisc	0.0001422	Paxs	700.88	Joback Method
dvisc	0.0001905	Paxs	652.36	Joback Method
dvisc	0.0002674	Paxs	603.84	Joback Method
dvisc	0.0003983	Paxs	555.33	Joback Method
dvisc	0.0006402	Paxs	506.81	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=U390291&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390291&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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