

# Succinic acid, 2,4,6-trichlorophenyl 2,2-dichloroethyl ester

<b>Inchi:</b>	InChI=1S/C12H9Cl5O4/c13-6-3-7(14)12(8(15)4-6)21-11(19)2-1-10(18)20-5-9(16)17/h3-4
<b>InchiKey:</b>	HXCWOHWTKOYSSS-UHFFFAOYSA-N
<b>Formula:</b>	C12H9Cl5O4
<b>SMILES:</b>	O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	394.46

## Physical Properties

Property code	Value	Unit	Source
gf	-396.25	kJ/mol	Joback Method
hf	-662.47	kJ/mol	Joback Method
hfus	42.75	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.679		Crippen Method
mcvol	232.260	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	2495.00		NIST Webbook
rinpol	2495.00		NIST Webbook
tb	854.87	K	Joback Method
tc	1086.74	K	Joback Method
tf	567.90	K	Joback Method
vc	0.886	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.11	J/mol×K	854.87	Joback Method
cpg	573.33	J/mol×K	1048.10	Joback Method
cpg	568.92	J/mol×K	1009.45	Joback Method
cpg	563.59	J/mol×K	970.81	Joback Method
cpg	557.35	J/mol×K	932.16	Joback Method
cpg	550.19	J/mol×K	893.52	Joback Method
cpg	576.82	J/mol×K	1086.74	Joback Method
dvisc	0.0000763	Paxs	854.87	Joback Method

dvisc	0.0000937	Paxs	807.04	Joback Method
dvisc	0.0001179	Paxs	759.21	Joback Method
dvisc	0.0001531	Paxs	711.38	Joback Method
dvisc	0.0002065	Paxs	663.56	Joback Method
dvisc	0.0002917	Paxs	615.73	Joback Method
dvisc	0.0004367	Paxs	567.90	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=U390527&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390527&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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