

# Succinic acid, 2,2-dichloroethyl 2-hexyl ester

<b>Inchi:</b>	InChI=1S/C12H20Cl2O4/c1-3-4-5-9(2)18-12(16)7-6-11(15)17-8-10(13)14/h9-10H,3-8H2,
<b>InchiKey:</b>	NMSHBDTUMFDEJK-UHFFFAOYSA-N
<b>Formula:</b>	C12H20Cl2O4
<b>SMILES:</b>	CCCCC(C)OC(=O)CCC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	299.19

## Physical Properties

Property code	Value	Unit	Source
gf	-446.42	kJ/mol	Joback Method
hf	-822.65	kJ/mol	Joback Method
hfus	33.76	kJ/mol	Joback Method
hvap	68.61	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.235		Crippen Method
mvol	219.300	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		NIST Webbook
tb	700.52	K	Joback Method
tc	892.04	K	Joback Method
tf	399.16	K	Joback Method
vc	0.842	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.07	J/mol×K	700.52	Joback Method
cpg	633.88	J/mol×K	860.12	Joback Method
cpg	623.41	J/mol×K	828.20	Joback Method
cpg	612.20	J/mol×K	796.28	Joback Method
cpg	600.25	J/mol×K	764.36	Joback Method
cpg	587.54	J/mol×K	732.44	Joback Method
cpg	643.60	J/mol×K	892.04	Joback Method
dvisc	0.0001058	Paxs	700.52	Joback Method

dvisc	0.0001408	Paxs	650.29	Joback Method
dvisc	0.0001967	Paxs	600.07	Joback Method
dvisc	0.0002919	Paxs	549.84	Joback Method
dvisc	0.0004692	Paxs	499.61	Joback Method
dvisc	0.0008385	Paxs	449.39	Joback Method
dvisc	0.0017341	Paxs	399.16	Joback Method

## Sources

<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=U390682&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390682&amp;Units=SI</a>
<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>

## 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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