

# Succinic acid, heptyl 2,3,4,6-tetrachlorophenyl ester

<b>Inchi:</b>	InChI=1S/C17H20Cl4O4/c1-2-3-4-5-6-9-24-13(22)7-8-14(23)25-17-12(19)10-11(18)15(20)
<b>InchiKey:</b>	PNUZRGUWPVKHQH-UHFFFAOYSA-N
<b>Formula:</b>	C17H20Cl4O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	430.15

## Physical Properties

Property code	Value	Unit	Source
gf	-349.41	kJ/mol	Joback Method
hf	-756.12	kJ/mol	Joback Method
hfus	54.63	kJ/mol	Joback Method
hvap	94.21	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.499		Crippen Method
mvol	290.470	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2764.00		NIST Webbook
rinpol	2764.00		NIST Webbook
tb	937.26	K	Joback Method
tc	1157.93	K	Joback Method
tf	621.85	K	Joback Method
vc	1.123	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.49	J/molxK	937.26	Joback Method
cpg	838.14	J/molxK	1121.15	Joback Method
cpg	832.01	J/molxK	1084.37	Joback Method
cpg	824.79	J/molxK	1047.59	Joback Method
cpg	816.47	J/molxK	1010.82	Joback Method
cpg	807.04	J/molxK	974.04	Joback Method
cpg	843.19	J/molxK	1157.93	Joback Method
dvisc	0.0000479	Paxs	937.26	Joback Method

dvisc	0.0000586	Paxs	884.69	Joback Method
dvisc	0.0000734	Paxs	832.12	Joback Method
dvisc	0.0000948	Paxs	779.56	Joback Method
dvisc	0.0001271	Paxs	726.99	Joback Method
dvisc	0.0001784	Paxs	674.42	Joback Method
dvisc	0.0002652	Paxs	621.85	Joback Method

## Sources

<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=U349679&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349679&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>
<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>

## 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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