

# Succinic acid, hexadecyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C22H39Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-28-20(26)16-17-21(27)
InchiKey:	GGIKVMZYWDHFFS-UHFFFAOYSA-N
Formula:	C22H39Cl3O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	473.90

## Physical Properties

Property code	Value	Unit	Source
gf	-366.43	kJ/mol	Joback Method
hf	-1042.98	kJ/mol	Joback Method
hfus	63.49	kJ/mol	Joback Method
hvap	94.74	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	7.704		Crippen Method
mvol	372.440	ml/mol	McGowan Method
pc	901.80	kPa	Joback Method
rinpol	2968.00		NIST Webbook
rinpol	2968.00		NIST Webbook
tb	964.40	K	Joback Method
tc	1181.25	K	Joback Method
tf	574.20	K	Joback Method
vc	1.452	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.72	J/molxK	964.40	Joback Method
cpg	1195.88	J/molxK	1000.54	Joback Method
cpg	1210.78	J/molxK	1036.68	Joback Method
cpg	1224.49	J/molxK	1072.83	Joback Method
cpg	1237.07	J/molxK	1108.97	Joback Method
cpg	1248.57	J/molxK	1145.11	Joback Method
cpg	1259.08	J/molxK	1181.25	Joback Method
dvisc	0.0002736	Paxs	574.20	Joback Method

dvisc	0.0001377	Paxs	639.23	Joback Method
dvisc	0.0000787	Paxs	704.27	Joback Method
dvisc	0.0000495	Paxs	769.30	Joback Method
dvisc	0.0000334	Paxs	834.33	Joback Method
dvisc	0.0000239	Paxs	899.37	Joback Method
dvisc	0.0000179	Paxs	964.40	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=U349179&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349179&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>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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