

# Succinic acid, 2,4,6-trichlorophenyl trans-hex-3-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C16H17Cl3O4/c1-2-3-4-5-8-22-14(20)6-7-15(21)23-16-12(18)9-11(17)10-13(16)
<b>InchiKey:</b>	GGDFTDJBWAFABU-ONEGZZNKSA-N
<b>Formula:</b>	C16H17Cl3O4
<b>SMILES:</b>	CCC=CCCOC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	379.66

## Physical Properties

Property code	Value	Unit	Source
gf	-256.05	kJ/mol	Joback Method
hf	-591.05	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.232		Crippen Method
mcvol	259.840	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2482.00		NIST Webbook
rinpol	2482.00		NIST Webbook
tb	876.13	K	Joback Method
tc	1096.52	K	Joback Method
tf	563.06	K	Joback Method
vc	0.999	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.67	J/molxK	876.13	Joback Method
cpg	738.99	J/molxK	1059.79	Joback Method
cpg	731.53	J/molxK	1023.06	Joback Method
cpg	723.20	J/molxK	986.32	Joback Method
cpg	713.96	J/molxK	949.59	Joback Method
cpg	703.79	J/molxK	912.86	Joback Method
cpg	745.58	J/molxK	1096.52	Joback Method
dvisc	0.0000558	Paxs	876.13	Joback Method

dvisc	0.0000689	Paxs	823.95	Joback Method
dvisc	0.0000876	Paxs	771.77	Joback Method
dvisc	0.0001153	Paxs	719.60	Joback Method
dvisc	0.0001584	Paxs	667.42	Joback Method
dvisc	0.0002296	Paxs	615.24	Joback Method
dvisc	0.0003567	Paxs	563.06	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U391124&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391124&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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