

# Succinic acid, propyl trans-hex-3-enyl ester

<b>Inchi:</b>	InChI=1S/C13H22O4/c1-3-5-6-7-11-17-13(15)9-8-12(14)16-10-4-2/h5-6H,3-4,7-11H2,1-2
<b>InchiKey:</b>	LDLIWNHOZGTWJR-AATRIKPKSA-N
<b>Formula:</b>	C13H22O4
<b>SMILES:</b>	CCC=CCCOC(=O)CCC(=O)OCCC
<b>Mol. weight [g/mol]:</b>	242.31

## Physical Properties

Property code	Value	Unit	Source
gf	-329.04	kJ/mol	Joback Method
hf	-684.03	kJ/mol	Joback Method
hfus	35.20	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.619		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
rinsol	1645.00		NIST Webbook
tb	653.58	K	Joback Method
tc	835.79	K	Joback Method
tf	375.51	K	Joback Method
vc	0.791	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.88	J/molxK	653.58	Joback Method
cpg	613.22	J/molxK	805.43	Joback Method
cpg	601.30	J/molxK	775.06	Joback Method
cpg	588.72	J/molxK	744.69	Joback Method
cpg	575.46	J/molxK	714.32	Joback Method
cpg	561.52	J/molxK	683.95	Joback Method
cpg	624.48	J/molxK	835.79	Joback Method
dvisc	0.0001162	Paxs	653.58	Joback Method
dvisc	0.0001511	Paxs	607.23	Joback Method

dvisc	0.0002051	Paxs	560.89	Joback Method
dvisc	0.0002942	Paxs	514.54	Joback Method
dvisc	0.0004533	Paxs	468.20	Joback Method
dvisc	0.0007681	Paxs	421.85	Joback Method
dvisc	0.0014825	Paxs	375.51	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=U353425&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353425&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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