

# Succinic acid, 2,2-dimethylpent-3-yl ethyl ester

<b>Inchi:</b>	InChI=1S/C13H24O4/c1-6-10(13(3,4)5)17-12(15)9-8-11(14)16-7-2/h10H,6-9H2,1-5H3
<b>InchiKey:</b>	ZFEZSBWPHYAIEC-UHFFFAOYSA-N
<b>Formula:</b>	C13H24O4
<b>SMILES:</b>	CCOC(=O)CCC(=O)OC(CC)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	244.33

## Physical Properties

Property code	Value	Unit	Source
gf	-408.86	kJ/mol	Joback Method
hf	-815.28	kJ/mol	Joback Method
hfus	24.06	kJ/mol	Joback Method
hvap	61.16	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.698		Crippen Method
mvol	208.910	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
tb	645.75	K	Joback Method
tc	832.89	K	Joback Method
tf	368.01	K	Joback Method
vc	0.794	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.62	J/molxK	645.75	Joback Method
cpg	587.54	J/molxK	676.94	Joback Method
cpg	602.64	J/molxK	708.13	Joback Method
cpg	616.93	J/molxK	739.32	Joback Method
cpg	630.43	J/molxK	770.51	Joback Method
cpg	643.16	J/molxK	801.70	Joback Method
cpg	655.14	J/molxK	832.89	Joback Method
dvisc	0.0021445	Paxs	368.01	Joback Method

dvisc	0.0009889	Paxs	414.30	Joback Method
dvisc	0.0005328	Paxs	460.59	Joback Method
dvisc	0.0003214	Paxs	506.88	Joback Method
dvisc	0.0002110	Paxs	553.17	Joback Method
dvisc	0.0001478	Paxs	599.46	Joback Method
dvisc	0.0001090	Paxs	645.75	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=U381729&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381729&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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