

# Succinic acid, 3-methylbut-2-en-1-yl 4-octyl ester

<b>Inchi:</b>	InChI=1S/C17H30O4/c1-5-7-9-15(8-6-2)21-17(19)11-10-16(18)20-13-12-14(3)4/h12,15H
<b>InchiKey:</b>	RFJQQECUBSLFLW-UHFFFAOYSA-N
<b>Formula:</b>	C17H30O4
<b>SMILES:</b>	CCCCC(CCC)OC(=O)CCC(=O)OCC=C(C)C
<b>Mol. weight [g/mol]:</b>	298.42

## Physical Properties

Property code	Value	Unit	Source
gf	-306.35	kJ/mol	Joback Method
hf	-781.66	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hvap	71.40	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.178		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	744.54	K	Joback Method
tc	929.10	K	Joback Method
tf	391.63	K	Joback Method
vc	1.010	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.43	J/mol×K	744.54	Joback Method
cpg	784.22	J/mol×K	775.30	Joback Method
cpg	800.11	J/mol×K	806.06	Joback Method
cpg	815.14	J/mol×K	836.82	Joback Method
cpg	829.32	J/mol×K	867.58	Joback Method
cpg	842.66	J/mol×K	898.34	Joback Method
cpg	855.19	J/mol×K	929.10	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U389557&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389557&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvp:</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>rinp:</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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