

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

<b>Inchi:</b>	InChI=1S/C15H26O4/c1-5-6-13(4)11-19-15(17)8-7-14(16)18-10-9-12(2)3/h9,13H,5-8,10-
<b>InchiKey:</b>	OPKRPJNPSDWCGK-UHFFFAOYSA-N
<b>Formula:</b>	C15H26O4
<b>SMILES:</b>	CCCC(C)COC(=O)CCC(=O)OCC=C(C)C
<b>Mol. weight [g/mol]:</b>	270.36

## Physical Properties

Property code	Value	Unit	Source
gf	-323.19	kJ/mol	Joback Method
hf	-740.38	kJ/mol	Joback Method
hfus	35.55	kJ/mol	Joback Method
hvap	66.95	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.255		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
tb	698.78	K	Joback Method
tc	883.94	K	Joback Method
tf	369.09	K	Joback Method
vc	0.898	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.83	J/mol×K	698.78	Joback Method
cpg	670.84	J/mol×K	729.64	Joback Method
cpg	686.03	J/mol×K	760.50	Joback Method
cpg	700.43	J/mol×K	791.36	Joback Method
cpg	714.04	J/mol×K	822.22	Joback Method
cpg	726.87	J/mol×K	853.08	Joback Method
cpg	738.96	J/mol×K	883.94	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=U389650&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389650&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

# 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>hvac:</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>rlnpol:</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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