

# Succinic acid, 3-methylbut-3-enyl propyl ester

<b>Inchi:</b>	InChI=1S/C12H20O4/c1-4-8-15-11(13)5-6-12(14)16-9-7-10(2)3/h2,4-9H2,1,3H3
<b>InchiKey:</b>	ZUJFYESWLQIMRW-UHFFFAOYSA-N
<b>Formula:</b>	C12H20O4
<b>SMILES:</b>	C=C(C)CCOC(=O)CCC(=O)OCCC
<b>Mol. weight [g/mol]:</b>	228.28

## Physical Properties

Property code	Value	Unit	Source
gf	-338.39	kJ/mol	Joback Method
hf	-664.97	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.229		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpola	1539.00		NIST Webbook
rinpola	1539.00		NIST Webbook
tb	623.10	K	Joback Method
tc	805.65	K	Joback Method
tf	353.60	K	Joback Method
vc	0.738	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.88	J/mol×K	623.10	Joback Method
cpg	508.04	J/mol×K	653.52	Joback Method
cpg	521.56	J/mol×K	683.95	Joback Method
cpg	534.43	J/mol×K	714.37	Joback Method
cpg	546.67	J/mol×K	744.80	Joback Method
cpg	558.27	J/mol×K	775.22	Joback Method
cpg	569.24	J/mol×K	805.65	Joback Method

# Sources

<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=U353439&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353439&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>

# 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>h vap:</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>r in pol:</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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