

# Succinic acid, 3,7-dimethyloct-6-en-1-yl isobutyl ester

<b>Inchi:</b>	InChI=1S/C18H32O4/c1-14(2)7-6-8-16(5)11-12-21-17(19)9-10-18(20)22-13-15(3)4/h7,15
<b>InchiKey:</b>	CWXJIOXASAI00N-UHFFFAOYSA-N
<b>Formula:</b>	C18H32O4
<b>SMILES:</b>	CC(C)=CCCC(C)CCOC(=O)CCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	312.44

## Physical Properties

Property code	Value	Unit	Source
gf	-300.37	kJ/mol	Joback Method
hf	-807.58	kJ/mol	Joback Method
hfus	39.80	kJ/mol	Joback Method
hvap	73.24	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.282		Crippen Method
mvol	275.060	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook
tb	766.98	K	Joback Method
tc	953.83	K	Joback Method
tf	387.90	K	Joback Method
vc	1.060	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.84	J/mol×K	766.98	Joback Method
cpg	843.16	J/mol×K	798.12	Joback Method
cpg	859.52	J/mol×K	829.26	Joback Method
cpg	874.94	J/mol×K	860.41	Joback Method
cpg	889.46	J/mol×K	891.55	Joback Method
cpg	903.09	J/mol×K	922.69	Joback Method
cpg	915.85	J/mol×K	953.83	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=U353336&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353336&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>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>rinpola:</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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