

# Succinic acid, 2,2-dichloroethyl 2-methyloct-5-yn-4-yl ester

Inchi:	InChI=1S/C15H22Cl2O4/c1-4-5-6-12(9-11(2)3)21-15(19)8-7-14(18)20-10-13(16)17/h11-
InchiKey:	UDLBQZQXXDBNQP-UHFFFAOYSA-N
Formula:	C15H22Cl2O4
SMILES:	CCC#CC(CC(C)C)OC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	337.24

## Physical Properties

Property code	Value	Unit	Source
gf	-220.80	kJ/mol	Joback Method
hf	-617.55	kJ/mol	Joback Method
hfus	41.13	kJ/mol	Joback Method
hvap	77.05	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.485		Crippen Method
mcvol	252.970	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpola	2034.00		NIST Webbook
rinpola	2034.00		NIST Webbook
tb	777.72	K	Joback Method
tc	983.72	K	Joback Method
tf	524.07	K	Joback Method
vc	0.966	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.00	J/molxK	777.72	Joback Method
cpg	704.20	J/molxK	812.05	Joback Method
cpg	717.46	J/molxK	846.39	Joback Method
cpg	729.76	J/molxK	880.72	Joback Method
cpg	741.13	J/molxK	915.05	Joback Method
cpg	751.56	J/molxK	949.38	Joback Method
cpg	761.07	J/molxK	983.72	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=U391027&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391027&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>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>rlnol:</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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