

# Benzeneacetic acid, 4-chloro-, 2,7-dimethyloct-1-en-3-yn-5-yl ester

<b>Inchi:</b>	InChI=1S/C18H21ClO2/c1-13(2)5-10-17(11-14(3)4)21-18(20)12-15-6-8-16(19)9-7-15/h6
<b>InchiKey:</b>	VYHJSUIXIQWEML-UHFFFAOYSA-N
<b>Formula:</b>	C18H21ClO2
<b>SMILES:</b>	<chem>C=C(C)C#CC(CC(C)C)OC(=O)Cc1ccc(Cl)cc1</chem>
<b>Mol. weight [g/mol]:</b>	304.81

## Physical Properties

Property code	Value	Unit	Source
gf	234.82	kJ/mol	Joback Method
hf	-72.95	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Joback Method
hvap	72.93	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.420		Crippen Method
mcvol	247.500	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
tb	761.30	K	Joback Method
tc	988.45	K	Joback Method
tf	494.02	K	Joback Method
vc	0.941	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.84	J/molxK	761.30	Joback Method
cpg	685.10	J/molxK	799.16	Joback Method
cpg	700.22	J/molxK	837.02	Joback Method
cpg	714.24	J/molxK	874.88	Joback Method
cpg	727.21	J/molxK	912.74	Joback Method
cpg	739.18	J/molxK	950.59	Joback Method
cpg	750.19	J/molxK	988.45	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=U407001&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407001&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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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