

# 4-Chlorobenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi:	InChI=1S/C17H19ClO2/c1-12(2)5-10-16(11-13(3)4)20-17(19)14-6-8-15(18)9-7-14/h6-9,1
InchiKey:	COCOCACCLBCEG-UHFFFAOYSA-N
Formula:	C17H19ClO2
SMILES:	<chem>C=C(C)C#CC(CC(C)C)OC(=O)c1ccc(Cl)cc1</chem>
Mol. weight [g/mol]:	290.79

## Physical Properties

Property code	Value	Unit	Source
gf	226.40	kJ/mol	Joback Method
hf	-52.31	kJ/mol	Joback Method
hfus	33.91	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.491		Crippen Method
mcvol	233.410	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tb	738.42	K	Joback Method
tc	969.47	K	Joback Method
tf	482.75	K	Joback Method
vc	0.884	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.06	J/mol×K	738.42	Joback Method
cpg	630.05	J/mol×K	776.93	Joback Method
cpg	644.90	J/mol×K	815.44	Joback Method
cpg	658.67	J/mol×K	853.94	Joback Method
cpg	671.39	J/mol×K	892.45	Joback Method
cpg	683.11	J/mol×K	930.96	Joback Method
cpg	693.88	J/mol×K	969.47	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>
<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=U299368&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299368&amp;Units=SI</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>rinp:</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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