

# Acetic acid, [2,3-dichloro-4-(2-methylene-1-oxobutyl)phenoxy] methyl ester

Other names: Ethacrynic acid, methyl ester  
Ethacrynic acid, methylated  
Acetic acid, 2-[2,3-dichloro-4-(2-methylene-1-oxobutyl)phenoxy]-, methyl ester  
Methyl ethacrylate

**Inchi:** InChI=1S/C14H14Cl2O4/c1-4-8(2)14(18)9-5-6-10(13(16)12(9)15)20-7-11(17)19-3/h5-6H

**InchiKey:** XFNMYPXAINMYAC-UHFFFAOYSA-N

**Formula:** C14H14Cl2O4

**SMILES:** C=C(CC)C(=O)c1ccc(OCC(=O)OC)c(Cl)c1Cl

**Mol. weight [g/mol]:** 317.17

**CAS:** 6463-21-4

## Physical Properties

Property code	Value	Unit	Source
gf	-261.89	kJ/mol	Joback Method
hf	-535.61	kJ/mol	Joback Method
hfus	36.27	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.694		Crippen Method
mcvol	219.420	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	785.34	K	Joback Method
tc	1005.59	K	Joback Method
tf	499.96	K	Joback Method
vc	0.840	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.64	J/molxK	785.34	Joback Method
cpg	573.25	J/molxK	822.05	Joback Method
cpg	583.94	J/molxK	858.76	Joback Method

cpg	593.74	J/mol×K	895.47	Joback Method
cpg	602.64	J/mol×K	932.18	Joback Method
cpg	610.66	J/mol×K	968.88	Joback Method
cpg	617.78	J/mol×K	1005.59	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=C6463214&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6463214&amp;Units=SI</a>
<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>

## 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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