

# Acetic acid, phenyl-, 3-hexenyl ester

<b>Other names:</b>	3-Hexenyl phenylacetate
<b>Inchi:</b>	InChI=1S/C14H18O2/c1-2-3-4-8-11-16-14(15)12-13-9-6-5-7-10-13/h3-7,9-10H,2,8,11-12
<b>InchiKey:</b>	FJKFIIYSBXHBCT-ONEGZZNKSA-N
<b>Formula:</b>	C14H18O2
<b>SMILES:</b>	CCC=CCCOC(=O)Cc1ccccc1
<b>Mol. weight [g/mol]:</b>	218.29

## Physical Properties

Property code	Value	Unit	Source
gf	25.71	kJ/mol	Joback Method
hf	-223.34	kJ/mol	Joback Method
hfus	29.05	kJ/mol	Joback Method
hvap	58.15	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.129		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1626.00		NIST Webbook
tb	626.85	K	Joback Method
tc	834.90	K	Joback Method
tf	341.04	K	Joback Method
vc	0.716	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.32	J/molxK	626.85	Joback Method
cpg	543.41	J/molxK	800.22	Joback Method
cpg	531.13	J/molxK	765.55	Joback Method
cpg	518.03	J/molxK	730.87	Joback Method
cpg	504.05	J/molxK	696.20	Joback Method
cpg	489.16	J/molxK	661.52	Joback Method
cpg	554.89	J/molxK	834.90	Joback Method
dvisc	0.0001300	Paxs	626.85	Joback Method

dvisc	0.0001691	Paxs	579.22	Joback Method
dvisc	0.0002307	Paxs	531.58	Joback Method
dvisc	0.0003345	Paxs	483.95	Joback Method
dvisc	0.0005261	Paxs	436.31	Joback Method
dvisc	0.0009243	Paxs	388.68	Joback Method
dvisc	0.0019011	Paxs	341.04	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U131737&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U131737&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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