

# 2-Heptenoic acid, phenyl ester

<b>Inchi:</b>	InChI=1S/C13H16O2/c1-2-3-4-8-11-13(14)15-12-9-6-5-7-10-12/h5-11H,2-4H2,1H3/b11-8
<b>InchiKey:</b>	BMPHWRUDHIZTMJ-DHZHZOJOSA-N
<b>Formula:</b>	C13H16O2
<b>SMILES:</b>	CCCCC=CC(=O)Oc1ccccc1
<b>Mol. weight [g/mol]:</b>	204.26

## Physical Properties

Property code	Value	Unit	Source
gf	17.29	kJ/mol	Joback Method
hf	-202.70	kJ/mol	Joback Method
hfus	26.46	kJ/mol	Joback Method
hvap	55.92	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.338		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
tb	603.97	K	Joback Method
tc	815.36	K	Joback Method
tf	329.77	K	Joback Method
vc	0.659	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.08	J/molxK	603.97	Joback Method
cpg	438.38	J/molxK	639.20	Joback Method
cpg	452.75	J/molxK	674.43	Joback Method
cpg	466.22	J/molxK	709.66	Joback Method
cpg	478.84	J/molxK	744.90	Joback Method
cpg	490.65	J/molxK	780.13	Joback Method
cpg	501.68	J/molxK	815.36	Joback Method
dvisc	0.0019948	Paxs	329.77	Joback Method

dvisc	0.0009848	Paxs	375.47	Joback Method
dvisc	0.0005667	Paxs	421.17	Joback Method
dvisc	0.0003633	Paxs	466.87	Joback Method
dvisc	0.0002522	Paxs	512.57	Joback Method
dvisc	0.0001858	Paxs	558.27	Joback Method
dvisc	0.0001434	Paxs	603.97	Joback Method

## Sources

<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=U406904&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406904&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>

## 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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