

# 5- METHYL-2- PHENYL-1- HEXANYL ACETATE

Inchi:	InChI=1S/C15H22O2/c1-12(2)9-10-15(11-17-13(3)16)14-7-5-4-6-8-14/h4-8,12,15H,9-11H
InchiKey:	SAVIONGKZKDADE-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CC(=O)OCC(CCC(C)C)c1ccccc1
Mol. weight [g/mol]:	234.33

## Physical Properties

Property code	Value	Unit	Source
gf	-50.97	kJ/mol	Joback Method
hf	-371.76	kJ/mol	Joback Method
hfus	24.39	kJ/mol	Joback Method
hvap	59.64	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.769		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
ripol	2029.00		NIST Webbook
ripol	2029.00		NIST Webbook
tb	644.69	K	Joback Method
tc	849.49	K	Joback Method
tf	327.39	K	Joback Method
vc	0.779	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.27	J/molxK	644.69	Joback Method
cpg	564.75	J/molxK	678.82	Joback Method
cpg	581.20	J/molxK	712.96	Joback Method
cpg	596.67	J/molxK	747.09	Joback Method
cpg	611.16	J/molxK	781.22	Joback Method
cpg	624.73	J/molxK	815.35	Joback Method
cpg	637.40	J/molxK	849.49	Joback Method
dvisc	0.0032184	Paxs	327.39	Joback Method

dvisc	0.0012640	Paxs	380.27	Joback Method
dvisc	0.0006237	Paxs	433.16	Joback Method
dvisc	0.0003589	Paxs	486.04	Joback Method
dvisc	0.0002302	Paxs	538.92	Joback Method
dvisc	0.0001598	Paxs	591.81	Joback Method
dvisc	0.0001178	Paxs	644.69	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=R389369&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R389369&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>

## 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>ripol:</b>	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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