

# 5-Phenylvaleric acid, isobutyl ester

<b>Inchi:</b>	InChI=1S/C15H22O2/c1-13(2)12-17-15(16)11-7-6-10-14-8-4-3-5-9-14/h3-5,8-9,13H,6-7,1
<b>InchiKey:</b>	AFNIRFWVAJKJEG-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O2
<b>SMILES:</b>	CC(C)COC(=O)CCCCc1ccccc1
<b>Mol. weight [g/mol]:</b>	234.33

## Physical Properties

Property code	Value	Unit	Source
gf	-48.53	kJ/mol	Joback Method
hf	-366.48	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.599		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
tb	645.13	K	Joback Method
tc	846.21	K	Joback Method
tf	342.39	K	Joback Method
vc	0.785	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.83	J/molxK	645.13	Joback Method
cpg	622.96	J/molxK	812.70	Joback Method
cpg	609.57	J/molxK	779.18	Joback Method
cpg	595.30	J/molxK	745.67	Joback Method
cpg	580.10	J/molxK	712.16	Joback Method
cpg	563.95	J/molxK	678.64	Joback Method
cpg	635.49	J/molxK	846.21	Joback Method
dvisc	0.0001267	Paxs	645.13	Joback Method

dvisc	0.0001684	Paxs	594.67	Joback Method
dvisc	0.0002360	Paxs	544.22	Joback Method
dvisc	0.0003541	Paxs	493.76	Joback Method
dvisc	0.0005830	Paxs	443.30	Joback Method
dvisc	0.0010907	Paxs	392.85	Joback Method
dvisc	0.0024547	Paxs	342.39	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=U406071&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406071&amp;Units=SI</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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