

# Benzenepropanoic acid 1-methylethyl ester

<b>Other names:</b>	3-Phenyl-propionic acid, isopropyl ester Isopropyl 3-phenylpropanoate
<b>Inchi:</b>	InChI=1S/C12H16O2/c1-10(2)14-12(13)9-8-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
<b>InchiKey:</b>	YQPAOLMOGAHRLG-UHFFFAOYSA-N
<b>Formula:</b>	C12H16O2
<b>SMILES:</b>	CC(C)OC(=O)CCc1ccccc1
<b>Mol. weight [g/mol]:</b>	192.25
<b>CAS:</b>	22767-95-9

## Physical Properties

Property code	Value	Unit	Source
gf	-73.79	kJ/mol	Joback Method
hf	-304.56	kJ/mol	Joback Method
hfus	20.14	kJ/mol	Joback Method
hvap	53.35	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.571		Crippen Method
mvol	163.620	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1385.00		NIST Webbook
tb	576.49	K	Joback Method
tc	786.80	K	Joback Method
tf	308.58	K	Joback Method
vc	0.618	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.41	J/molxK	576.49	Joback Method
cpg	463.49	J/molxK	751.74	Joback Method
cpg	451.37	J/molxK	716.69	Joback Method
cpg	438.42	J/molxK	681.64	Joback Method
cpg	424.63	J/molxK	646.59	Joback Method
cpg	409.96	J/molxK	611.54	Joback Method

cpg	474.82	J/molxK	786.80	Joback Method
dvisc	0.0001725	Paxs	576.49	Joback Method
dvisc	0.0002268	Paxs	531.84	Joback Method
dvisc	0.0003136	Paxs	487.19	Joback Method
dvisc	0.0004628	Paxs	442.54	Joback Method
dvisc	0.0007455	Paxs	397.88	Joback Method
dvisc	0.0013546	Paxs	353.23	Joback Method
dvisc	0.0029260	Paxs	308.58	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=C22767959&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22767959&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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