

# 3-Phenylpropionic acid, 3-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C16H16O2/c1-13-6-5-9-15(12-13)18-16(17)11-10-14-7-3-2-4-8-14/h2-9,12H,10
<b>InchiKey:</b>	BOGCCTWRSGWVMV-UHFFFAOYSA-N
<b>Formula:</b>	C16H16O2
<b>SMILES:</b>	Cc1cccc(OC(=O)CCc2ccccc2)c1
<b>Mol. weight [g/mol]:</b>	240.30

## Physical Properties

Property code	Value	Unit	Source
gf	65.11	kJ/mol	Joback Method
hf	-156.78	kJ/mol	Joback Method
hfus	27.68	kJ/mol	Joback Method
hvap	65.58	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.533		Crippen Method
mvol	196.220	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1922.00		NIST Webbook
rinpol	1922.00		NIST Webbook
tb	700.11	K	Joback Method
tc	933.89	K	Joback Method
tf	407.60	K	Joback Method
vc	0.740	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.98	J/molxK	700.11	Joback Method
cpg	533.95	J/molxK	739.07	Joback Method
cpg	548.72	J/molxK	778.04	Joback Method
cpg	562.33	J/molxK	817.00	Joback Method
cpg	574.82	J/molxK	855.96	Joback Method
cpg	586.26	J/molxK	894.92	Joback Method
cpg	596.69	J/molxK	933.89	Joback Method
dvisc	0.0011644	Paxs	407.60	Joback Method

dvisc	0.0006540	Paxs	456.35	Joback Method
dvisc	0.0004106	Paxs	505.10	Joback Method
dvisc	0.0002798	Paxs	553.86	Joback Method
dvisc	0.0002029	Paxs	602.61	Joback Method
dvisc	0.0001544	Paxs	651.36	Joback Method
dvisc	0.0001220	Paxs	700.11	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=U307780&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307780&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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