

# (3-Methoxy-4-isopropoxy-phenyl)-propionic acid, methyl ester

Inchi:	InChI=1S/C14H20O4/c1-10(2)18-12-7-5-11(9-13(12)16-3)6-8-14(15)17-4/h5,7,9-10H,6,8
InchiKey:	LXMIJFMUCVNRKF-UHFFFAOYSA-N
Formula:	C14H20O4
SMILES:	COC(=O)CCc1ccc(OC(C)C)c(OC)c1
Mol. weight [g/mol]:	252.31

## Physical Properties

Property code	Value	Unit	Source
gf	-286.21	kJ/mol	Joback Method
hf	-633.22	kJ/mol	Joback Method
hfus	26.92	kJ/mol	Joback Method
hvap	63.95	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.588		Crippen Method
mvol	203.540	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	1710.50		NIST Webbook
rinpol	1710.50		NIST Webbook
tb	677.05	K	Joback Method
tc	879.11	K	Joback Method
tf	400.62	K	Joback Method
vc	0.765	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.23	J/molxK	677.05	Joback Method
cpg	563.88	J/molxK	710.73	Joback Method
cpg	578.68	J/molxK	744.40	Joback Method
cpg	592.62	J/molxK	778.08	Joback Method
cpg	605.67	J/molxK	811.76	Joback Method
cpg	617.84	J/molxK	845.44	Joback Method
cpg	629.12	J/molxK	879.11	Joback Method
dvisc	0.0008086	Paxs	400.62	Joback Method

dvisc	0.0004578	Paxs	446.69	Joback Method
dvisc	0.0002882	Paxs	492.76	Joback Method
dvisc	0.0001964	Paxs	538.84	Joback Method
dvisc	0.0001422	Paxs	584.91	Joback Method
dvisc	0.0001079	Paxs	630.98	Joback Method
dvisc	0.0000850	Paxs	677.05	Joback Method

## Sources

<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=R158066&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R158066&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>
<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>

## 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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