

# (4-Isopropoxy-phenyl)-acetic acid, methyl ester

Inchi:	InChI=1S/C12H16O3/c1-9(2)15-11-6-4-10(5-7-11)8-12(13)14-3/h4-7,9H,8H2,1-3H3
InchiKey:	IXIIOTCCONXDNO-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	COC(=O)Cc1ccc(OC(C)C)cc1
Mol. weight [g/mol]:	208.25

## Physical Properties

Property code	Value	Unit	Source
gf	-188.42	kJ/mol	Joback Method
hf	-448.25	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	56.42	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.189		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinsol	1489.40		NIST Webbook
tb	603.89	K	Joback Method
tc	812.91	K	Joback Method
tf	343.33	K	Joback Method
vc	0.635	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.73	J/molxK	603.89	Joback Method
cpg	434.72	J/molxK	638.73	Joback Method
cpg	448.90	J/molxK	673.56	Joback Method
cpg	462.28	J/molxK	708.40	Joback Method
cpg	474.87	J/molxK	743.24	Joback Method
cpg	486.66	J/molxK	778.07	Joback Method
cpg	497.67	J/molxK	812.91	Joback Method
dvisc	0.0015703	Paxs	343.33	Joback Method
dvisc	0.0008297	Paxs	386.76	Joback Method

dvisc	0.0004986	Paxs	430.18	Joback Method
dvisc	0.0003290	Paxs	473.61	Joback Method
dvisc	0.0002328	Paxs	517.04	Joback Method
dvisc	0.0001738	Paxs	560.46	Joback Method
dvisc	0.0001353	Paxs	603.89	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=R158100&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R158100&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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