

# m-Methoxybenzoic acid, 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C17H18O4/c1-12(2)20-15-9-4-5-10-16(15)21-17(18)13-7-6-8-14(11-13)19-3/h4
InchiKey:	CDBFQNMZHZHGSBJ-UHFFFAOYSA-N
Formula:	C17H18O4
SMILES:	COc1cccc(C(=O)Oc2ccccc2OC(C)C)c1
Mol. weight [g/mol]:	286.32

## Physical Properties

Property code	Value	Unit	Source
gf	-148.54	kJ/mol	Joback Method
hf	-458.61	kJ/mol	Joback Method
hfus	28.73	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.702		Crippen Method
mcvol	222.050	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1985.40		NIST Webbook
rinpol	1985.40		NIST Webbook
tb	772.37	K	Joback Method
tc	1000.99	K	Joback Method
tf	460.85	K	Joback Method
vc	0.826	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.08	J/molxK	772.37	Joback Method
cpg	689.41	J/molxK	962.89	Joback Method
cpg	679.05	J/molxK	924.78	Joback Method
cpg	667.44	J/molxK	886.68	Joback Method
cpg	654.59	J/molxK	848.58	Joback Method
cpg	640.47	J/molxK	810.47	Joback Method
cpg	698.52	J/molxK	1000.99	Joback Method
dvisc	0.0000600	Paxs	772.37	Joback Method

dvisc	0.0000760	Paxs	720.45	Joback Method
dvisc	0.0000998	Paxs	668.53	Joback Method
dvisc	0.0001371	Paxs	616.61	Joback Method
dvisc	0.0001998	Paxs	564.69	Joback Method
dvisc	0.0003143	Paxs	512.77	Joback Method
dvisc	0.0005475	Paxs	460.85	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=U292631&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292631&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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