

# Benzene, 1-methoxy-4-methyl-2-(1-methylethyl)-

<b>Other names:</b>	2-Isopropyl-1-methoxy-4-methylbenzene Isothymol methyl ether Anisole, 2-isopropyl-4-methyl- 2-isopropyl-4-methylanisole
<b>Inchi:</b>	InChI=1S/C11H16O/c1-8(2)10-7-9(3)5-6-11(10)12-4/h5-8H,1-4H3
<b>InchiKey:</b>	CVUAHQAHQICPSF-UHFFFAOYSA-N
<b>Formula:</b>	C11H16O
<b>SMILES:</b>	COc1ccc(C)cc1C(C)C
<b>Mol. weight [g/mol]:</b>	164.24
<b>CAS:</b>	31574-44-4

## Physical Properties

Property code	Value	Unit	Source
gf	27.45	kJ/mol	Joback Method
hf	-194.28	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	45.70	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.127		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1215.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1595.00		NIST Webbook
tb	509.70	K	Joback Method
tc	716.96	K	Joback Method
tf	272.42	K	Joback Method
vc	0.555	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.70	J/molxK	509.70	Joback Method
cpg	342.03	J/molxK	544.24	Joback Method
cpg	356.63	J/molxK	578.79	Joback Method
cpg	370.54	J/molxK	613.33	Joback Method
cpg	383.76	J/molxK	647.87	Joback Method
cpg	396.29	J/molxK	682.41	Joback Method
cpg	408.15	J/molxK	716.96	Joback Method
dvisc	0.0018910	Paxs	272.42	Joback Method
dvisc	0.0009689	Paxs	311.97	Joback Method
dvisc	0.0005771	Paxs	351.51	Joback Method
dvisc	0.0003817	Paxs	391.06	Joback Method
dvisc	0.0002723	Paxs	430.61	Joback Method
dvisc	0.0002057	Paxs	470.15	Joback Method
dvisc	0.0001623	Paxs	509.70	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=C31574444&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31574444&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>ripol:</b>	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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