

# Benzene, 1-(2-methoxy-1-propenyl)-3-methyl-, (Z)-

Inchi:	InChI=1S/C11H14O/c1-9-5-4-6-11(7-9)8-10(2)12-3/h4-8H,1-3H3/b10-8+
InchiKey:	IKQRYJRRRCQHMOX-CSKARUKUSA-N
Formula:	C11H14O
SMILES:	<chem>COC(C)=Cc1cccc(C)c1</chem>
Mol. weight [g/mol]:	162.23
CAS:	101948-73-6

## Physical Properties

Property code	Value	Unit	Source
gf	111.19	kJ/mol	Joback Method
hf	-70.10	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	45.47	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.002		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	509.20	K	Joback Method
tc	724.36	K	Joback Method
tf	255.86	K	Joback Method
vc	0.542	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.38	J/mol×K	509.20	Joback Method
cpg	323.47	J/mol×K	545.06	Joback Method
cpg	337.73	J/mol×K	580.92	Joback Method
cpg	351.19	J/mol×K	616.78	Joback Method
cpg	363.86	J/mol×K	652.64	Joback Method
cpg	375.80	J/mol×K	688.50	Joback Method
cpg	387.02	J/mol×K	724.36	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C101948736&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C101948736&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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