

# 2-Methoxybenzyl alcohol, tert.-butyl ether

<b>Inchi:</b>	InChI=1S/C12H18O2/c1-12(2,3)14-9-10-7-5-6-8-11(10)13-4/h5-8H,9H2,1-4H3
<b>InchiKey:</b>	USKWAFXHSMRYOH-UHFFFAOYSA-N
<b>Formula:</b>	C12H18O2
<b>SMILES:</b>	COc1ccccc1COC(C)(C)C
<b>Mol. weight [g/mol]:</b>	194.27

## Physical Properties

Property code	Value	Unit	Source
gf	-54.22	kJ/mol	Joback Method
hf	-339.14	kJ/mol	Joback Method
hfus	15.45	kJ/mol	Joback Method
hvap	48.77	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.010		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinsol	1393.00		NIST Webbook
tb	547.23	K	Joback Method
tc	756.39	K	Joback Method
tf	310.82	K	Joback Method
vc	0.625	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.69	J/molxK	547.23	Joback Method
cpg	418.50	J/molxK	582.09	Joback Method
cpg	434.39	J/molxK	616.95	Joback Method
cpg	449.38	J/molxK	651.81	Joback Method
cpg	463.50	J/molxK	686.67	Joback Method
cpg	476.78	J/molxK	721.53	Joback Method
cpg	489.24	J/molxK	756.39	Joback Method
dvisc	0.0017989	Paxs	310.82	Joback Method
dvisc	0.0009020	Paxs	350.22	Joback Method

dvisc	0.0005200	Paxs	389.62	Joback Method
dvisc	0.0003317	Paxs	429.02	Joback Method
dvisc	0.0002282	Paxs	468.43	Joback Method
dvisc	0.0001664	Paxs	507.83	Joback Method
dvisc	0.0001270	Paxs	547.23	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U378197&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U378197&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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