

# Benzeneethanol, 3-methoxy-

<b>Other names:</b>	Phenethyl alcohol, m-methoxy- m-Methoxyphenethyl alcohol m-Methoxyphenylethanol 1-(2-Hydroxyethyl)-3-methoxybenzene 2-(3-Methoxyphenyl)ethanol 3-Methoxyphenethyl alcohol
<b>Inchi:</b>	InChI=1S/C9H12O2/c1-11-9-4-2-3-8(7-9)5-6-10/h2-4,7,10H,5-6H2,1H3
<b>InchiKey:</b>	UPPGEJSCUZMCMW-UHFFFAOYSA-N
<b>Formula:</b>	C9H12O2
<b>SMILES:</b>	COc1cccc(CCO)c1
<b>Mol. weight [g/mol]:</b>	152.19
<b>CAS:</b>	5020-41-7

## Physical Properties

Property code	Value	Unit	Source
gf	-114.14	kJ/mol	Joback Method
hf	-288.48	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	57.66	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.230		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1235.00		NIST Webbook
tb	551.58	K	Joback Method
tc	746.03	K	Joback Method
tf	313.18	K	Joback Method
vc	0.469	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.51	J/molxK	551.58	Joback Method
cpg	300.67	J/molxK	583.99	Joback Method

cpg	311.28	J/molxK	616.40	Joback Method
cpg	321.36	J/molxK	648.80	Joback Method
cpg	330.92	J/molxK	681.21	Joback Method
cpg	339.96	J/molxK	713.62	Joback Method
cpg	348.51	J/molxK	746.03	Joback Method
dvisc	0.0055162	Paxs	313.18	Joback Method
dvisc	0.0018885	Paxs	352.91	Joback Method
dvisc	0.0008032	Paxs	392.65	Joback Method
dvisc	0.0003997	Paxs	432.38	Joback Method
dvisc	0.0002237	Paxs	472.11	Joback Method
dvisc	0.0001370	Paxs	511.85	Joback Method
dvisc	0.0000901	Paxs	551.58	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.20	K	1.60	NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5020417&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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