Benzene, (1-methoxyethyl)-

Other names:	Ether, methyl «alpha»-methylbenzyl «alpha»-Methylbenzyl methyl ether (1-Methoxyethyl)benzene Methyl «alpha»-phenethyl ether 1-Methoxy-1-phenylethane 1-Phenylethyl methyl ether
Inchi:	InChI=1S/C9H12O/c1-8(10-2)9-6-4-3-5-7-9/h3-8H,1-2H3
InchiKey:	PLKSMSKTENNPEJ-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	COC(C)c1ccccc1
Mol. weight [g/mol]:	136.19
CAS:	4013-34-7

Physical Properties

Property code	Value	Unit	Source
gf	29.87	kJ/mol	Joback Method
hf	-130.06	kJ/mol	Joback Method
hfus	10.77	kJ/mol	Joback Method
hvap	49.10 ± 0.40	kJ/mol	NIST Webbook
log10ws	-2.24		Crippen Method
logp	2.394		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	453.98	K	Joback Method
tc	664.69	K	Joback Method
tf	224.84	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.41	J/mol×K	664.69	Joback Method
cpg	238.66	J/mol×K	453.98	Joback Method
cpg	252.69	J/mol×K	489.10	Joback Method

cpg	266.01	J/mol×K	524.22	Joback Method
cpg	278.62	J/mol×K	559.33	Joback Method
cpg	290.55	J/mol×K	594.45	Joback Method
cpg	301.80	J/mol×K	629.57	Joback Method
dvisc	0.0001942	Pa×s	453.98	Joback Method
dvisc	0.0040329	Pa×s	224.84	Joback Method
dvisc	0.0016853	Pa×s	263.03	Joback Method
dvisc	0.0008786	Pa×s	301.22	Joback Method
dvisc	0.0005304	Pa×s	339.41	Joback Method
dvisc	0.0003546	Pa×s	377.60	Joback Method
dvisc	0.0002553	Pa×s	415.79	Joback Method
hvapt	49.20 ± 0.40	kJ/mol	305.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4013347&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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