

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	312.41	J/mol×K	664.69	Joback Method
dvisc	0.0040329	Paxs	224.84	Joback Method
dvisc	0.0016853	Paxs	263.03	Joback Method
dvisc	0.0008786	Paxs	301.22	Joback Method
dvisc	0.0005304	Paxs	339.41	Joback Method
dvisc	0.0003546	Paxs	377.60	Joback Method
dvisc	0.0002553	Paxs	415.79	Joback Method
dvisc	0.0001942	Paxs	453.98	Joback Method
hvapt	49.20 ± 0.40	kJ/mol	305.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4013347&Units=SI
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

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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