Benzene, (methoxymethyl)-

Other names:	Ether, benzyl methyl
	«alpha»-Methoxytoluene
	Benzyl methyl ether
	Methyl benzyl ether
	Methoxymethylbenzene
	«alpha»-Methylbenzyl ether
Inchi:	InChI=1S/C8H10O/c1-9-7-8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	GQKZBCPTCWJTAS-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	COCc1ccccc1
Mol. weight [g/mol]:	122.16
CAS:	538-86-3

Physical Properties

Property code	Value	Unit	Source
affp	816.70	kJ/mol	NIST Webbook
basg	787.50	kJ/mol	NIST Webbook
gf	23.89	kJ/mol	Joback Method
hf	-104.14	kJ/mol	Joback Method
hfus	11.70	kJ/mol	Joback Method
hvap	51.40 ± 0.30	kJ/mol	NIST Webbook
ie	9.12	eV	NIST Webbook
ie	8.83 ± 0.05	eV	NIST Webbook
ie	8.85 ± 0.03	eV	NIST Webbook
ie	9.07	eV	NIST Webbook
ie	8.76	eV	NIST Webbook
log10ws	-1.86		Crippen Method
logp	1.833		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	973.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	966.10		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	981.00		NIST Webbook
ripol	1377.00		NIST Webbook

ripol	1396.00		NIST Webbook
ripol	1391.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1377.00		NIST Webbook
tb	440.95 ± 0.40	K	NIST Webbook
tb	443.65 ± 0.50	K	NIST Webbook
tb	443.70 ± 0.60	K	NIST Webbook
tb	447.00	K	NIST Webbook
tc	639.91	K	Joback Method
tf	220.52 ± 0.40	K	NIST Webbook
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.15	J/mol×K	431.54	Joback Method
cpg	254.14	J/mol×K	605.18	Joback Method
cpg	244.12	J/mol×K	570.45	Joback Method
cpg	233.52	J/mol×K	535.73	Joback Method
cpg	222.34	J/mol×K	501.00	Joback Method
cpg	210.55	J/mol×K	466.27	Joback Method
cpg	263.60	J/mol×K	639.91	Joback Method
dvisc	0.0002090	Pa×s	431.54	Joback Method
dvisc	0.0002657	Pa×s	397.71	Joback Method
dvisc	0.0003534	Pa×s	363.88	Joback Method
dvisc	0.0004982	Pa×s	330.06	Joback Method
dvisc	0.0007596	Pa×s	296.23	Joback Method
dvisc	0.0012913	Pa×s	262.40	Joback Method
dvisc	0.0025685	Pa×s	228.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.50 ± 1.50	K	4.00	NIST Webbook
tbrp	339.00 ± 4.00	K	2.00	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=C538863&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume