Benzene, 1-methoxy-4-methyl-

Other names:	1-Methyl-4-methoxybenzene
	1-methoxy-4-methylbenzene
	4-Methyl-1-methoxybenzene
	4-Methylmethoxybenzene
	4-Methylphenol methyl ether
	4-methoxymethylbenzene
	4-methoxytoluene
	4-methylanisole
	Methyl 4-methylphenyl ether
	Methyl p-cresyl ether
	NSC 6254
	anisole, p-methyl-
	methyl 4-tolyl ether
	methyl p-methylphenyl ether
	methyl p-tolyl ether
	p-Cresyl methyl ether
	p-Methylanisol
	p-cresol methyl ether
	p-methoxytoluene
	p-methylanisole
	p-tolyl methyl ether
	para-Methyl anisol
	para-Methyl anisole
	toluene, 4-methoxy-
Inchi:	InChI=1S/C8H10O/c1-7-3-5-8(9-2)6-4-7/h3-6H,1-2H3
InchiKey:	CHLICZRVGGXEOD-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	COc1ccc(C)cc1
Mol. weight [g/mol]:	122.16
CAS:	104-93-8

Physical Properties

Property code	Value	Unit	Source
affp	841.00 ± 8.00	kJ/mol	NIST Webbook
basg	809.00 ± 8.00	kJ/mol	NIST Webbook
gf	14.26	kJ/mol	Joback Method

hf	-115.61	kJ/mol	Joback Method
hfus	11.32	kJ/mol	Joback Method
hvap	38.75	kJ/mol	Joback Method
ie	7.90 ± 0.03	eV	NIST Webbook
ie	7.85	eV	NIST Webbook
ie	7.83	eV	NIST Webbook
ie	8.30 ± 0.10	eV	NIST Webbook
ie	7.90 ± 0.05	eV	NIST Webbook
ie	8.14 ± 0.01	eV	NIST Webbook
ie	8.18	eV	NIST Webbook
ie	8.17	eV	NIST Webbook
ie	8.16	eV	NIST Webbook
ie	7.91	eV	NIST Webbook
ie	8.00 ± 0.15	eV	NIST Webbook
log10ws	-2.07		Crippen Method
logp	2.004		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
rinpol	1003.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	999.20		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1029.50		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	986.60		NIST Webbook
rinpol	1005.00		NIST Webbook

rinpol	1004.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	999.20		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1029.50		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	986.60		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
ripol	1461.10		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1446.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1461.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1446.00		NIST Webbook
ripol	1441.00		NIST Webbook
tb	450.90 ± 3.00	K	NIST Webbook
tb	449.90 ± 0.50	K	NIST Webbook
tb	449.70 ± 0.20	K	NIST Webbook
tb	443.75 ± 0.50	K	NIST Webbook
tb	447.20	K	NIST Webbook
tc	666.00 ± 1.00	K	NIST Webbook
tf	241.96 ± 0.30	K	NIST Webbook
tf	241.10 ± 0.30	K	NIST Webbook
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.01	J/mol×K	436.52	Joback Method
cpg	210.91	J/mol×K	471.49	Joback Method
cpg	222.27	J/mol×K	506.47	Joback Method

cpg	233.10	J/mol×K	541.44	Joback Method
cpg	243.40	J/mol×K	576.41	Joback Method
cpg	253.17	J/mol×K	611.38	Joback Method
cpg	262.44	J/mol×K	646.36	Joback Method
dvisc	0.0017292	Pa×s	241.09	Joback Method
dvisc	0.0009715	Pa×s	273.66	Joback Method
dvisc	0.0006170	Pa×s	306.23	Joback Method
dvisc	0.0004276	Pa×s	338.81	Joback Method
dvisc	0.0003160	Pa×s	371.38	Joback Method
dvisc	0.0002453	Pa×s	403.95	Joback Method
dvisc	0.0001977	Pa×s	436.52	Joback Method
pvap	0.04	kPa	278.80	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.03	kPa	276.40	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.03	kPa	277.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.03	kPa	275.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.05	kPa	281.70	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.06	kPa	284.80	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.08	kPa	287.50	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study

pvap	0.09	kPa	289.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.10	kPa	290.40	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.10	kPa	291.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.10	kPa	291.30	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.13	kPa	294.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.14	kPa	296.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.16	kPa	297.10	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.18	kPa	299.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.19	kPa	300.10	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.20	kPa	300.10	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study

pvap	0.21	kPa	301.10	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.25	kPa	303.10	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.28	kPa	305.00	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.34	kPa	308.00	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study

Sources

Ternary liquid-liquid equilibrium: Nitric acid - water - anisole/4-methyl anisole:	https://www.doi.org/10.1016/j.fluid.2011.10.022
Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study:	https://www.doi.org/10.1016/j.jct.2015.02.001
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=C104938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume