Benzene, 1-methoxy-2-methyl-

Other names:	1-methoxy-2-methylbenzene
	2-Methylmethoxybenzene
	2-methoxymethylbenzene
	2-methoxytoluene
	2-methyl-1-methoxybenzene
	2-methylanisole
	Methyl-o-cresol
	NSC 6253
	anisole, o-methyl-
	methyl 2-tolyl ether
	methyl o-cresyl ether
	methyl o-methylphenyl ether
	methyl o-tolyl ether
	o-Methylanisol
	o-cresol methyl ether
	o-cresyl methyl ether
	o-methoxytoluene
	o-methylanisole
	toluene, o-methoxy-
Inchi:	InChI=1S/C8H10O/c1-7-5-3-4-6-8(7)9-2/h3-6H,1-2H3
InchiKey:	DTFKRVXLBCAIOZ-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	COc1ccccc1C
Mol. weight [g/mol]:	122.16
CAS:	578-58-5

Physical Properties

Property code	Value	Unit	Source
affp	850.00 ± 8.00	kJ/mol	NIST Webbook
basg	818.00 ± 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	8.03 ± 0.02	eV	NIST Webbook
ie	8.24	eV	NIST Webbook
ie	8.24	eV	NIST Webbook

ie	7.90	eV	NIST Webbook
ie	8.10 ± 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	1013.50		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1013.50		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	983.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1390.00		NIST Webbook
tb	444.20	K	NIST Webbook
tb	445.00 ± 0.50	K	NIST Webbook
tb	444.88 ± 0.30	K	NIST Webbook
tb	557.35 ± 1.00	K	NIST Webbook
tc	662.00 ± 0.60	K	NIST Webbook
tf	238.97 ± 0.30	K	NIST Webbook
tf	239.05 ± 0.50	K	NIST Webbook
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.44	J/mol×K	646.36	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	199.01	J/mol×K	436.52	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	0.35	kPa	308.00	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.29	kPa	305.10	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.26	kPa	303.30	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.21	kPa	300.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.21	kPa	300.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study

pvap	0.18	kPa	298.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.16	kPa	296.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.13	kPa	293.40	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.10	kPa	290.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.08	kPa	286.80	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.07	kPa	285.70	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.06	kPa	282.60	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.05	kPa	280.60	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.04	kPa	278.70	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.04	kPa	277.70	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study

pvap	0.04	kPa	275.80	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C578585&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
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