Benzene, 1-methoxy-3-methyl-

Other names:	1-Methyl-3-methoxybenzene 1-methoxy-3-methylbenzene 3-Methyl-1-methoxybenzene 3-Methylmethoxybenzene 3-methoxymethylbenzene 3-methoxytoluene 3-methylanisole Methyl 3-methylphenyl ether Methyl m-cresyl ether NSC 6255 anisole, m-methyl- m-cresol methyl ether m-cresyl methyl ether m-methoxytoluene m-methylanisole methyl 3-tolyl ether methyl m-tolyl ether toluene, 3-methoxy-
Inchi:	InChI=1S/C8H10O/c1-7-4-3-5-8(6-7)9-2/h3-6H,1-2H3
InchiKey:	OSIGJGFTADMDOB-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	COc1cccc(C)c1
Mol. weight [g/mol]:	122.16
CAS:	100-84-5

Physical Properties

Property code	Value	Unit	Source
affp	860.00 ± 8.00	kJ/mol	NIST Webbook
basg	828.00 ± 8.00	kJ/mol	NIST Webbook
chl	-4421.90	kJ/mol	NIST Webbook
gf	14.26	kJ/mol	Joback Method
hf	-115.61	kJ/mol	Joback Method
hfl	-155.40	kJ/mol	NIST Webbook
hfus	11.32	kJ/mol	Joback Method
hvap	38.75	kJ/mol	Joback Method
ie	8.31 ± 0.05	eV	NIST Webbook
ie	8.10 ± 0.15	eV	NIST Webbook

ie	8.00	eV	NIST Webbook
ie	8.40 ± 0.10	eV	NIST Webbook
ie	8.28	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	1020.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	999.10		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1029.60		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1430.00		NIST Webbook
tb	449.90 ± 0.50	K	NIST Webbook
tb	448.70	K	NIST Webbook
tb	448.50 ± 0.50	K	NIST Webbook
tb	449.70 ± 0.50	K	NIST Webbook
tb	449.59 ± 0.20	K	NIST Webbook
tc	665.30 ± 0.60	K	NIST Webbook
tf	217.23 ± 0.40	K	NIST Webbook
tf	217.90 ± 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	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
cpg	210.91	J/mol×K	471.49	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	0.0017292	Pa×s	241.09	Joback Method
dvisc	0.0001977	Pa×s	436.52	Joback Method
pvap	0.41	kPa	312.20	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.34	kPa	310.00	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.30	kPa	308.00	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.24	kPa	305.00	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.23	kPa	304.10	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.18	kPa	301.10	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.14	kPa	297.70	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.09	kPa	291.90	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.08	kPa	289.40	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study

pvap	0.05	kPa	284.70	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.04	kPa	280.60	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.03	kPa	277.80	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study
pvap	0.03	kPa	276.70	Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100845&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

Latest version available from:

https://www.chemeo.com/cid/28-910-0/Benzene-1-methoxy-3-methyl.pdf

Generated by Cheméo on 2024-10-12 03:09:31.476542609 +0000 UTC m=+3283434.113511860.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.