Benzene, 1-chloro-4-methoxy-

Other names:	1-Chloro-4-methoxybenzene
	1-Methoxy-4-chlorobenzene
	4-Chloroanisole
	4-Chlorophenol methyl ether
	Anisole, p-chloro-
	Anisyl chloride
	NSC 4129
	p-Chloroanisole
	p-Chloromethoxybenzene
	p-Chlorophenyl methyl ether
	p-Methoxychlorobenzene
	p-chloroanisol
	para-Chloroanisole
Inchi:	InChI=1S/C7H7ClO/c1-9-7-4-2-6(8)3-5-7/h2-5H,1H3
InchiKey:	YRGAYAGBVIXNAQ-UHFFFAOYSA-N
Formula:	C7H7ClO
SMILES:	COc1ccc(Cl)cc1
Mol. weight [g/mol]:	142.58
CAS:	623-12-1

Physical Properties

Property code	Value	Unit	Source
gf	-6.09	kJ/mol	Joback Method
hf	-110.71	kJ/mol	Joback Method
hfus	12.92	kJ/mol	Joback Method
hvap	54.80 ± 0.80	kJ/mol	NIST Webbook
ie	8.18	eV	NIST Webbook
ie	7.79	eV	NIST Webbook
ie	8.25 ± 0.03	eV	NIST Webbook
ie	8.25 ± 0.15	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
log10ws	-2.78		Estimated Solubility Method
log10ws	-2.78		Aqueous Solubility Prediction Method
logp	2.349		Crippen Method
mcvol	103.840	ml/mol	McGowan Method

pc	3773.04	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1079.50		NIST Webbook
rinpol	1123.50		NIST Webbook
rinpol	1131.70		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1131.70		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1090.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1592.00		NIST Webbook
tb	473.20	K	NIST Webbook
tc	670.60	K	Joback Method
tf	259.74	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.68	J/mol×K	451.07	Joback Method
cpg	230.02	J/mol×K	634.01	Joback Method
cpg	221.95	J/mol×K	597.42	Joback Method
cpg	213.38	J/mol×K	560.84	Joback Method
cpg	204.32	J/mol×K	524.25	Joback Method
cpg	194.76	J/mol×K	487.66	Joback Method
cpg	237.62	J/mol×K	670.60	Joback Method
dvisc	0.0002283	Pa×s	451.07	Joback Method
dvisc	0.0002817	Pa×s	419.18	Joback Method
dvisc	0.0003597	Pa×s	387.29	Joback Method
dvisc	0.0004800	Pa×s	355.41	Joback Method
dvisc	0.0006780	Pa×s	323.52	Joback Method

dvisc	0.0010328	Pa×s	291.63	Joback Method
dvisc	0.0017445	Pa×s	259.74	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume