Benzene, 1-chloro-4-methoxy-2-methyl-

Other names: Benzene, 1-chloro-2-methyl-4-methoxy
4-Chloro-3-methylanisole
Inchi: InChI=1S/C8H9ClO/c1-6-5-7(10-2)3-4-8(6)9/h3-5H,1-2H3
InchiKey: SDGMUBWPXBSKCT-UHFFFAOYSA-N
Formula: C8H9ClO
SMILES: COc1ccc(Cl)c(C)c1
Mol. weight [g/mol]: 156.61
CAS: 13334-71-9

Physical Properties

Property code	Value	Unit	Source
gf	-7.30	kJ/mol	Joback Method
hf	-142.82	kJ/mol	Joback Method
hfus	15.12	kJ/mol	Joback Method
hvap	43.80	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.657		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
rinpol	1180.00		NIST Webbook
rinpol	1224.50		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1224.50		NIST Webbook
tb	478.93	K	Joback Method
tc	696.56	K	Joback Method
tf	283.53	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.28	J/mol×K	478.93	Joback Method
cpg	235.27	J/mol×K	515.20	Joback Method
cpg	245.75	J/mol×K	551.47	Joback Method

cpg	255.72	J/mol×K	587.74	Joback Method
cpg	265.18	J/mol×K	624.02	Joback Method
cpg	274.14	J/mol×K	660.29	Joback Method
cpg	282.59	J/mol×K	696.56	Joback Method
dvisc	0.0013423	Pa×s	283.53	Joback Method
dvisc	0.0008406	Pa×s	316.10	Joback Method
dvisc	0.0005745	Pa×s	348.66	Joback Method
dvisc	0.0004190	Pa×s	381.23	Joback Method
dvisc	0.0003212	Pa×s	413.80	Joback Method
dvisc	0.0002559	Pa×s	446.36	Joback Method
dvisc	0.0002103	Pa×s	478.93	Joback Method

Sources

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=C13334719&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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