

2-Chloro-5-methylphenol, methyl ether

Other names:	Benzene, 1-chloro-4-methyl-2-methoxy
Inchi:	InChI=1S/C8H9ClO/c1-6-3-4-7(9)8(5-6)10-2/h3-5H,1-2H3
InchiKey:	KBRLTYHUJDMMLI-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	COc1cc(C)ccc1Cl
Mol. weight [g/mol]:	156.61
CAS:	73909-16-7

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	1237.40		NIST Webbook
tb	478.93	K	Joback Method
tc	696.56	K	Joback Method
tf	283.53	K	Joback Method
vc	0.443	m ³ /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	Paxs	283.53	Joback Method
dvisc	0.0008406	Paxs	316.10	Joback Method
dvisc	0.0005745	Paxs	348.66	Joback Method
dvisc	0.0004190	Paxs	381.23	Joback Method
dvisc	0.0003212	Paxs	413.80	Joback Method
dvisc	0.0002559	Paxs	446.36	Joback Method
dvisc	0.0002103	Paxs	478.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73909167&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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

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