4-Chloro-2-methoxyphenol, acetate

Inchi: InChI=1S/C9H9ClO3/c1-6(11)13-8-4-3-7(10)5-9(8)12-2/h3-5H,1-2H3
InchiKey: QGTPWFVCCNXPON-UHFFFAOYSA-N
Formula: C9H9ClO3
SMILES: COc1cc(Cl)ccc1OC(C)=O
Mol. weight [g/mol]: 200.62

Physical Properties

Property code	Value	Unit	Source
gf	-232.80	kJ/mol	Joback Method
hf	-408.26	kJ/mol	Joback Method
hfus	20.50	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.274		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	1436.60		NIST Webbook
tb	578.10	K	Joback Method
tc	798.52	K	Joback Method
tf	366.96	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.40	J/mol×K	578.10	Joback Method
cpg	352.12	J/mol×K	761.78	Joback Method
cpg	343.37	J/mol×K	725.05	Joback Method
cpg	334.01	J/mol×K	688.31	Joback Method
cpg	324.06	J/mol×K	651.57	Joback Method
cpg	313.52	J/mol×K	614.84	Joback Method
cpg	360.25	J/mol×K	798.52	Joback Method
dvisc	0.0001811	Pa×s	578.10	Joback Method
dvisc	0.0002203	Pa×s	542.91	Joback Method

dvisc	0.0002755	Pa×s	507.72	Joback Method
dvisc	0.0003562	Pa×s	472.53	Joback Method
dvisc	0.0004798	Pa×s	437.34	Joback Method
dvisc	0.0006811	Pa×s	402.15	Joback Method
dvisc	0.0010339	Pa×s	366.96	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U352854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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