Formic acid, (4-chloro-2-methoxyphenyl)methyl ester

Inchi: InChI=1S/C9H9ClO3/c1-12-9-4-8(10)3-2-7(9)5-13-6-11/h2-4,6H,5H2,1H3

InchiKey: KZQCTTJBDTWLDC-UHFFFAOYSA-N

Formula: C9H9ClO3

SMILES: COc1cc(Cl)ccc1COC=O

Mol. weight [g/mol]: 200.62

Physical Properties

Property code	Value	Unit	Source
gf	-203.40	kJ/mol	Joback Method
hf	-381.26	kJ/mol	Joback Method
hfus	21.19	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.022		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
tb	572.89	K	Joback Method
tc	788.23	K	Joback Method
tf	359.03	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.70	J/mol×K	572.89	Joback Method
cpg	314.50	J/mol×K	608.78	Joback Method
cpg	324.76	J/mol×K	644.67	Joback Method
cpg	334.46	J/mol×K	680.56	Joback Method
cpg	343.60	J/mol×K	716.45	Joback Method
cpg	352.17	J/mol×K	752.34	Joback Method
cpg	360.16	J/mol×K	788.23	Joback Method
dvisc	0.0011578	Pa×s	359.03	Joback Method

dvisc	0.0007556	Pa×s	394.67	Joback Method
dvisc	0.0005292	Pa×s	430.32	Joback Method
dvisc	0.0003914	Pa×s	465.96	Joback Method
dvisc	0.0003021	Pa×s	501.60	Joback Method
dvisc	0.0002414	Pa×s	537.25	Joback Method
dvisc	0.0001983	Pa×s	572.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368241&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