2-Chloropropionic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C9H7Cl3O2/c1-5(10)9(13)14-6-2-3-7(11)8(12)4-6/h2-5H,1H3
InchiKey: YFMJDVKPXPSLOQ-UHFFFAOYSA-N
Formula: C9H7Cl3O2
SMILES: CC(Cl)C(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 253.51

Physical Properties

Property code	Value	Unit	Source
gf	-154.10	kJ/mol	Joback Method
hf	-312.80	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	61.15	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.526		Crippen Method
mcvol	158.070	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	630.10	K	Joback Method
tc	865.66	K	Joback Method
tf	389.57	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.21	J/mol×K	630.10	Joback Method
cpg	335.13	J/mol×K	669.36	Joback Method
cpg	344.34	J/mol×K	708.62	Joback Method
cpg	352.87	J/mol×K	747.88	Joback Method
cpg	360.71	J/mol×K	787.14	Joback Method
cpg	367.88	J/mol×K	826.40	Joback Method
cpg	374.40	J/mol×K	865.66	Joback Method
dvisc	0.0013740	Pa×s	389.57	Joback Method

dvisc	0.0008493	Pa×s	429.66	Joback Method
dvisc	0.0005698	Pa×s	469.75	Joback Method
dvisc	0.0004071	Pa×s	509.84	Joback Method
dvisc	0.0003055	Pa×s	549.92	Joback Method
dvisc	0.0002383	Pa×s	590.01	Joback Method
dvisc	0.0001919	Pa×s	630.10	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=U307755&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