2-[2-Chlorophenyl]propenoic acid

Inchi: InChI=1S/C10H9ClO2/c1-7(6-10(12)13)8-4-2-3-5-9(8)11/h2-6H,1H3,(H,12,13)/b7-6-
InchiKey: MPYCDNZCWADMHD-SREVYHEPSA-N
Formula: C9H7ClO2
SMILES: CC(=CC(=O)O)c1ccccc1Cl
Mol. weight [g/mol]: 182.60
CAS: 4513-41-1

Physical Properties

Property code	Value	Unit	Source
gf	-69.90	kJ/mol	Joback Method
hf	-197.79	kJ/mol	Joback Method
hfus	24.08	kJ/mol	Joback Method
hvap	68.64	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.828		Crippen Method
mcvol	143.380	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	647.38	K	Joback Method
tc	863.97	K	Joback Method
tf	363.03	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.79	J/mol×K	647.38	Joback Method
cpg	337.49	J/mol×K	683.48	Joback Method
cpg	346.50	J/mol×K	719.58	Joback Method
cpg	354.89	J/mol×K	755.67	Joback Method
cpg	362.70	J/mol×K	791.77	Joback Method
cpg	369.98	J/mol×K	827.87	Joback Method
cpg	376.76	J/mol×K	863.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4513411&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume