2-(3-Chlorophenoxy)propionic acid

Other names:	(dl) 2-(m-chlorophenoxy)propanoic acid
	2-(3-Chlorophenoxy)propanoic acid
	2-(m-Chlorophenoxy)propionic acid
	3-CPA
	3CP
	Cloprop
	Fruitone CPA
	Metachlorphenprop
	Propanoic acid, 2-(3-chlorophenoxy)-
	Propionic acid, 2-(m-chlorophenoxy)-
	dl-2-(3-Chlorophenoxy)propionic acid
	dl-2-(m-Chlorophenoxy)propionic acid
	«alpha»-(3-Chlorophenoxy)propionic acid
	Â«alphaÂ»-(3-Chlorophenoxy)propionic acid
Inchi:	InChI=1S/C9H9ClO3/c1-6(9(11)12)13-8-4-2-3-7(10)5-8/h2-6H,1H3,(H,11,12)
InchiKey:	YNTJKQDWYXUTLZ-UHFFFAOYSA-N
Formula:	C9H9ClO3
SMILES:	CC(Oc1cccc(Cl)c1)C(=O)O
Mol. weight [g/mol]:	200.62
CAS:	101-10-0

Physical Properties

Property code	Value	Unit	Source
gf	-257.43	kJ/mol	Joback Method
hf	-422.08	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	68.40	kJ/mol	Joback Method
log10ws	-2.22		Aqueous Solubility Prediction Method
logp	2.192		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	642.44	K	Joback Method
tc	852.38	K	Joback Method
tf	378.03	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.00	J/mol×K	642.44	Joback Method
cpg	335.62	J/mol×K	677.43	Joback Method
cpg	344.62	J/mol×K	712.42	Joback Method
cpg	353.03	J/mol×K	747.41	Joback Method
cpg	360.85	J/mol×K	782.40	Joback Method
cpg	368.09	J/mol×K	817.39	Joback Method
cpg	374.77	J/mol×K	852.38	Joback Method
dvisc	0.0026543	Pa×s	378.03	Joback Method
dvisc	0.0010273	Pa×s	422.10	Joback Method
dvisc	0.0004758	Pa×s	466.17	Joback Method
dvisc	0.0002517	Pa×s	510.24	Joback Method
dvisc	0.0001473	Pa×s	554.30	Joback Method
dvisc	0.0000933	Pa×s	598.37	Joback Method
dvisc	0.0000629	Pa×s	642.44	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C101100&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume