2-(O-CHLOROPHENOXY)PROPIONIC ACID

Other names: 2-(2-Chlorophenoxy)propanoic acid
Acide (o-chlorophenoxy)-2 propionique
Propionic acid, 2-(o-chlorophenoxy)-
Inchi: InChI=1S/C9H9ClO3/c1-6(9(11)12)13-8-5-3-2-4-7(8)10/h2-6H,1H3,(H,11,12)
InchiKey: ZGWNXHRVUJVMCP-UHFFFAOYSA-N
Formula: C9H9ClO3
SMILES: CC(Oc1ccccc1Cl)C(=O)O
Mol. weight [g/mol]: 200.62

Physical Properties

Property code	Value	Unit	Source
hfus	20.27	kJ/mol	Joback Method
hvap	84.67	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-2.22		Aqueous Solubility Prediction Method
logp	2.192		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
tb	539.98	K	Cheméo Relay (1.0)
tf	386.65	K	Aqueous Solubility Prediction 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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25140867&Units=SI

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

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point