

Propanoic acid, 2-(2-chlorophenoxy)-

Other names:	2-(2-Chlorophenoxy)propanoic acid 2-(o-Chlorophenoxy)propionic 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
CAS:	25140-86-7

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
mvol	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	386.65	K	Aqueous Solubility Prediction Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.00	J/molxK	642.44	Joback Method
cpg	368.09	J/molxK	817.39	Joback Method
cpg	360.85	J/molxK	782.40	Joback Method

cpg	353.03	J/molxK	747.41	Joback Method
cpg	344.62	J/molxK	712.42	Joback Method
cpg	335.62	J/molxK	677.43	Joback Method
cpg	374.77	J/molxK	852.38	Joback Method
dvisc	0.0000629	Paxs	642.44	Joback Method
dvisc	0.0000933	Paxs	598.37	Joback Method
dvisc	0.0001473	Paxs	554.30	Joback Method
dvisc	0.0002517	Paxs	510.24	Joback Method
dvisc	0.0004758	Paxs	466.17	Joback Method
dvisc	0.0010273	Paxs	422.10	Joback Method
dvisc	0.0026543	Paxs	378.03	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

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

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method:

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

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

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

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