o-Chlorophenoxyacetic acid

Other names:	2-(2-chlorophenoxy)acetic acid
	2-Chlorophenoxyacetic acid
	Acetic acid, (2-chlorophenoxy)-
	Acetic acid, (o-chlorophenoxy)-
	Acide o-chlorophenoxyacetique
Inchi:	InChI=1S/C8H7ClO3/c9-6-3-1-2-4-7(6)12-5-8(10)11/h1-4H,5H2,(H,10,11)
InchiKey:	OPQYFNRLWBWCST-UHFFFAOYSA-N
Formula:	C8H7ClO3
SMILES:	O=C(O)COc1ccccc1Cl
Mol. weight [g/mol]:	186.59
CAS:	614-61-9

Physical Properties

Property code	Value	Unit	Source
gf	-263.41	kJ/mol	Joback Method
hf	-396.16	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	66.56	kJ/mol	Joback Method
log10ws	-2.16		Aqueous Solubility Prediction Method
logp	1.803		Crippen Method
mcvol	125.370	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
tb	620.00	K	Joback Method
tc	829.16	K	Joback Method
tf	422.40	K	Aqueous Solubility Prediction Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.94	J/mol×K	620.00	Joback Method
cpg	316.43	J/mol×K	794.30	Joback Method

cpg	309.96	J/mol×K	759.44	Joback Method
cpg	302.98	J/mol×K	724.58	Joback Method
cpg	295.49	J/mol×K	689.72	Joback Method
cpg	287.49	J/mol×K	654.86	Joback Method
cpg	322.41	J/mol×K	829.16	Joback Method
dvisc	0.0000801	Pa×s	620.00	Joback Method
dvisc	0.0001153	Pa×s	580.29	Joback Method
dvisc	0.0001753	Pa×s	540.59	Joback Method
dvisc	0.0002846	Pa×s	500.88	Joback Method
dvisc	0.0005023	Pa×s	461.17	Joback Method
dvisc	0.0009866	Pa×s	421.47	Joback Method
dvisc	0.0022303	Pa×s	381.76	Joback Method

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C614619&Units=SI

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