Acetic acid, (4-chlorophenoxy)-

Other names:	(4-Chlorophenoxy)acetic acid
	(p-Chlorophenoxy)acetic acid
	2-(4-chlorophenoxy)acetic acid
	4-CP
	4-CPA
	Acetic acid, (p-chlorophenoxy)-
	Acetic acid, 2-(4-chlorophenoxy)-
	BI 12
	CPA
	Kyselina 4-chlorfenoxyoctova
	Marks 4-cpa
	NSC 8769
	PCPA
	Sure-Set
	Tomato Fix
	Tomato Fix concentrate
	Tomato hold
	Tomatotone
	para-Chlorophenoxyacetic acid
Inchi:	InChI=1S/C8H7ClO3/c9-6-1-3-7(4-2-6)12-5-8(10)11/h1-4H,5H2,(H,10,11)
InchiKey:	SODPIMGUZLOIPE-UHFFFAOYSA-N
Formula:	C8H7ClO3
SMILES:	O=C(O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	186.59
CAS:	122-88-3

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	-2.29		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	434.65	K	Aqueous Solubility Prediction Method
tf	431.48 ± 0.20	K	NIST Webbook
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	278.94	J/mol×K	620.00	Joback Method
cpg	322.41	J/mol×K	829.16	Joback Method
dvisc	0.0022303	Pa×s	381.76	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
hfust	36.27	kJ/mol	429.60	NIST Webbook
hfust	36.27	kJ/mol	429.60	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C122883&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
hfust:	Enthalpy of fusion at a given temperature
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