4-Chlorophenoxyacetic acid

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

Physical Properties

Property code	Value	Unit	Source
hf	-467.30	kJ/mol	Cheméo Relay (1.0)
hfus	21.20	kJ/mol	Joback Method
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-2.29		Aqueous Solubility Prediction Method
logp	1.803		Crippen Method
mcvol	125.370	ml/mol	McGowan Method
tb	567.54	K	Cheméo Relay (1.0)
tf	434.65	K	Aqueous Solubility Prediction Method

tf	431.48 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.94	J/mol×K	620.00	Joback Method
cpg	287.49	J/mol×K	654.86	Joback Method
cpg	295.49	J/mol×K	689.72	Joback Method
cpg	302.98	J/mol×K	724.58	Joback Method
cpg	309.96	J/mol×K	759.44	Joback Method
cpg	316.43	J/mol×K	794.30	Joback Method
cpg	322.41	J/mol×K	829.16	Joback Method
dvisc	0.0022303	Pa×s	381.76	Joback Method
dvisc	0.0009866	Pa×s	421.47	Joback Method
dvisc	0.0005023	Pa×s	461.17	Joback Method
dvisc	0.0002846	Pa×s	500.88	Joback Method
dvisc	0.0001753	Pa×s	540.59	Joback Method
dvisc	0.0001153	Pa×s	580.29	Joback Method
dvisc	0.0000801	Pa×s	620.00	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
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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C122883&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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