Fenoprop

Other names:
(.+/-.)-2-(2,4,5-Trichlorophenoxy)propanoic acid
(.+/-.)-Fenoprop
(.+/-.)-Silvex
2,4,5-TC
2,4,5-TCPPA
2,4,5-TP
2,4,5-Trichlorophenoxy-«alpha»-propionic acid
2,4,5-Trichlorophenoxy-Â«alphaÂ»-propionic acid
2-(2,4,5-Trichloor-fenoxy)-propionzuur
2-(2,4,5-Trichlor-phenoxy)-propionsaeure
2-(2,4,5-Trichlorophenoxy)propanoic acid
2-(2,4,5-Trichlorophenoxy)propionic acid
Acide 2-(2,4,5-trichloro-phenoxy) propionique
Acido 2-(2,4,5-tricloro-fenossi)-propionico
Amchem 2,4,5-TP
Aqua-vex
Color-Set
Double strength
Fenormone
Fruitone T
Herbicides, silvex
Kuran
Kurosal
Kurosal G
Kwas 2,4,5-trojchlorofenoksypropionowy
Kyselina 2-(2,4,5-trichlorfenoxy)propionova
Miller nu set
Propanoic acid, 2-(2,4,5-trichlorophenoxy)-
Propionic acid, 2-(2,4,5-trichlorophenoxy)-
Propon
Rcra waste number U233
Silvex
Silvex acid
Silvi-Rhap
Sta-fast
«alpha»-(2,4,5-Trichlorophenoxy)propionic acid
Â«alphaÂ»-(2,4,5-Trichlorophenoxy)propionic acid

Inchi: InChI=1S/C9H7Cl3O3/c1-4(9(13)14)15-8-3-6(11)5(10)2-7(8)12/h2-4H,1H3,(H,13,14)

InchiKey: ZLSWBLPERHFHIS-UHFFFAOYSA-N

Formula: C9H7Cl3O3

SMILES: CC(Oc1cc(Cl)c(Cl)cc1Cl)C(=O)O
Mol. weight [g/mol]: 269.51
CAS: 93-72-1

Physical Properties

Property code	Value	Unit	Source
gf	-300.55	kJ/mol	Joback Method
hf	-476.50	kJ/mol	Joback Method
hfus	27.88	kJ/mol	Joback Method
hvap	78.49	kJ/mol	Joback Method
log10ws	-3.55		Aqueous Solubility Prediction Method
logp	3.499		Crippen Method
mcvol	163.940	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1869.00		NIST Webbook
tb	727.26	K	Joback Method
tc	945.37	K	Joback Method
tf	453.81 ± 0.20	K	NIST Webbook
tf	451.68	K	Aqueous Solubility Prediction Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.14	J/mol×K	945.37	Joback Method
cpg	363.09	J/mol×K	727.26	Joback Method
cpg	370.85	J/mol×K	763.61	Joback Method
cpg	378.03	J/mol×K	799.96	Joback Method
cpg	384.65	J/mol×K	836.32	Joback Method
cpg	390.70	J/mol×K	872.67	Joback Method
cpg	396.19	J/mol×K	909.02	Joback Method
dvisc	0.0000422	Pa×s	727.26	Joback Method
dvisc	0.0007580	Pa×s	462.91	Joback Method
dvisc	0.0003801	Pa×s	506.97	Joback Method
dvisc	0.0002128	Pa×s	551.03	Joback Method
dvisc	0.0001298	Pa×s	595.09	Joback Method

dvisc	0.0000848	Pa×s	639.14	Joback Method
dvisc	0.0000585	Pa×s	683.20	Joback Method
hfust	39.58	kJ/mol	450.60	NIST Webbook

Sources

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=C93721&Units=SI

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

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

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume