Dichlorprop

Other names:

(.+/-.)-2,4-DP
(.+/-.)-2-(2,4-Dichlorophenoxy)propanoic acid
(.+/-.)-2-(2,4-Dichlorophenoxy)propionic acid
(.+/-.)-Dichlorprop
2,4-DP
2,4-Dichlorophenoxy-«alpha»-propionic acid
2,4-Dichlorophenoxy-Â«alphaÂ»-propionic acid
2-(2,4-DP)
2-(2,4-Dichloor-fenoxy)-propionzuur
2-(2,4-Dichlor-phenoxy)-propionsaeure
2-(2,4-Dichlorophenoxy)propanoic acid
2-(2,4-Dichlorophenoxy)propionic acid
AF 302
Acide 2-(2,4-dichloro-phenoxy)propionique
Acido 2-(2,4-dicloro-fenossi)-propionico
Alpha-(2,4-dichlorophenoxy)propionic acid
BH 2,4-DP
Canapur DP
Celatox-DP
Cornox RK
Cornox rd
Desormone
Dichloroprop
Hedonal DP
Herbizid DP
Hormatox
Kildip
Kwas 2,4-dwuchlorofenoksypropionowy
Kyselina 2-(2,4-dichlorfenoxy)propionova
MSS 2,4-DP
NSC 39624
Polyclene
Polymone
Polytox
Propanoic acid, 2-(2,4-dichlorophenoxy)-
Propionic acid, 2-(2,4-dichlorophenoxy)-
RD 406
Seritox 50
U46 DP-FLUID
Weedone 170

	Weedone DP
	«alpha»-(2,4-Dichlorophenoxy)propionic acid
	Â«alphaÂ»-(2,4-Dichlorophenoxy)propionic acid
Inchi:	InChI=1S/C9H8Cl2O3/c1-5(9(12)13)14-8-3-2-6(10)4-7(8)11/h2-5H,1H3,(H,12,13)
InchiKey:	MZHCENGPTKEIGP-UHFFFAOYSA-N
Formula:	C9H8Cl2O3
SMILES:	CC(Oc1ccc(Cl)cc1Cl)C(=O)O
Mol. weight [g/mol]:	235.06
CAS:	120-36-5

Physical Properties

Property code	Value	Unit	Source
gf	-278.99	kJ/mol	Joback Method
hf	-449.29	kJ/mol	Joback Method
hfus	24.08	kJ/mol	Joback Method
hsub	130.00 ± 3.00	kJ/mol	NIST Webbook
hsub	116.00 ± 6.00	kJ/mol	NIST Webbook
hvap	73.44	kJ/mol	Joback Method
log10ws	-2.83		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.45		Aqueous Solubility Prediction Method
logp	2.845		Crippen Method
mcvol	151.700	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1756.00		NIST Webbook
tb	684.85	K	Joback Method
tc	899.03	K	Joback Method
tf	390.90	K	Aqueous Solubility Prediction Method
tf	389.90 ± 0.20	K	NIST Webbook
tf	389.64 ± 0.20	K	NIST Webbook
tf	389.70	K	Standard Sublimation Enthalpies of some dichlorophenoxy acids and their methyl esters
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.97	J/mol×K	863.33	Joback Method
cpg	369.69	J/mol×K	791.94	Joback Method
cpg	362.19	J/mol×K	756.24	Joback Method
cpg	354.11	J/mol×K	720.55	Joback Method
cpg	345.44	J/mol×K	684.85	Joback Method
cpg	376.61	J/mol×K	827.63	Joback Method
cpg	388.78	J/mol×K	899.03	Joback Method
dvisc	0.0013532	Pa×s	420.47	Joback Method
dvisc	0.0000516	Pa×s	684.85	Joback Method
dvisc	0.0000738	Pa×s	640.79	Joback Method
dvisc	0.0001112	Pa×s	596.72	Joback Method
dvisc	0.0001789	Pa×s	552.66	Joback Method
dvisc	0.0003124	Pa×s	508.60	Joback Method
dvisc	0.0006065	Pa×s	464.53	Joback Method
hfust	32.00	kJ/mol	391.30	NIST Webbook
hfust	30.43	kJ/mol	389.20	NIST Webbook
hsubt	128.00 ± 2.00	kJ/mol	359.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120365&Units=SI

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

Standard Sublimation Enthalpies of some dichlorophenoxy acids and their methyl esters: https://www.doi.org/10.1021/je049626l

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

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

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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