2,4-D

Other names:

(2,4-Dichloor-fenoxy)-azijnzuur
(2,4-Dichlor-phenoxy)-essigsaeure
(2,4-Dichlorophenoxy)acetic acid
(2,4-Dichlorophenyloxy)acetic acid
(2,4-Dichlorphenoxy)acetic acid
(Dichlorophenoxy)acetic acid
2,4-D Acid
2,4-D Mecoprop
2,4-Dichlorophenoxyethanoic acid
2,4-Dwuchlorofenoksyoctowy kwas
2,4-dichlorophenoxyacetic acid
94-75-7
Acetic acid, (2,4-dichlorophenoxy)-
Acide 2,4-dichloro phenoxyacetique
Acido(2,4-dicloro-fenossi)-acetico
Acme LV 4
Acme amine 4
Acme butyl ester 4
Agrotect
Amidox
Aminopielik 50SL
Amoxone
Atlas D
B-Selektonon
BH 2,4-D
Barrage HF
Brush-rhap
Chipco turf herbicide "D"
Chloroxone
Crop rider
Crotilin
D 50
DMA-4
Dacamine
Debroussaillant 600
Decamine
Ded-Weed LV-69
Desormone
Dezormon
Diclordon

Dicopur
Dicotox
Dinoxol
Dormone
ENT 8,538
Emulsamine E-3
Emulsamine bk
Envert 171
Envert dt
Esteron
Esteron 44 weed killer
Esteron 76 BE
Esteron 99
Esteron 99 concentrate
Esteron brush killer
Esterone
Esterone four
Estone
Farmco
Fernesta
Fernimine
Fernoxone
Ferxone
Foredex 75
Formula 40
Hedonal
Hedonal, herbicide
Herbidal
Huragan
Ipaner
Kwas 2,4-dwuchlorofenoksyoctowy
Kwasu 2,4-dwuchlorofenoksyoctowego
Kyselina 2,4-dichlorfenoxyoctova
Lawn-keep
Macrondray
Miracle
Monosan
Mota Maskros
Moxone
NSC 423
Netagrone
Netagrone 600
Pennamine

Pennamine D
Phenox
Pielik
Planotox
Plantgard
RCRA waste number U240
Rhodia
Salvo
Spritz-hormin/2,4-D
Spritz-hormit/2,4-D
Super D weedone
Superormone concentre
Tiller S
Transamine
Tributon
Trinoxol
U 46
U 46DP
U-5043
Uniso
Vergemaster
Verton
Verton 2D
Verton D
Vertron 2D
Vidon 638
Visko-rhap
Visko-rhap low drift herbicides
Visko-rhap low volatile 4l
Weed tox
Weed-B-gon
Weed-Rhap
Weed-ag-bar
Weedar
Weedar-64
Weedatul
Weedez wonder bar
Weedone
Weedone LV4
Weedtrol
dichlorophenoxyacetic acid
ethanoic acid, 2,4-dichlorophenoxy-

Inchi: InChI=1S/C8H6Cl2O3/c9-5-1-2-7(6(10)3-5)13-4-8(11)12/h1-3H,4H2,(H,11,12)

InchiKey:	OVSKIKFHRZPJSS-UHFFFAOYSA-N
Formula:	C8H6Cl2O3
SMILES:	O=C(O)COc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	221.04
CAS:	94-75-7

Physical Properties

Property code	Value	Unit	Source
gf	-284.97	kJ/mol	Joback Method
hf	-423.37	kJ/mol	Joback Method
hfus	25.01	kJ/mol	Joback Method
hsub	125.00 ± 3.00	kJ/mol	NIST Webbook
hsub	115.00 ± 6.00	kJ/mol	NIST Webbook
hvap	71.61	kJ/mol	Joback Method
log10ws	-2.51		Aqueous Solubility Prediction Method
logp	2.457		Crippen Method
mcvol	137.610	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1702.00		NIST Webbook
tb	662.41	K	Joback Method
tc	875.98	K	Joback Method
tf	412.80 ± 0.20	K	NIST Webbook
tf	411.98	K	Aqueous Solubility Prediction Method
tf	414.50	K	Standard Sublimation Enthalpies of some dichlorophenoxy acids and their methyl esters
tf	412.65 ± 0.20	K	NIST Webbook
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.64	J/mol×K	840.39	Joback Method
cpg	318.83	J/mol×K	769.20	Joback Method
cpg	312.19	J/mol×K	733.60	Joback Method
cpg	305.04	J/mol×K	698.01	Joback Method

cpg	297.39	J/mol×K	662.41	Joback Method
cpg	324.98	J/mol×K	804.79	Joback Method
cpg	335.82	J/mol×K	875.98	Joback Method
dvisc	0.0012073	Pa×s	424.20	Joback Method
dvisc	0.0000662	Pa×s	662.41	Joback Method
dvisc	0.0000920	Pa×s	622.71	Joback Method
dvisc	0.0001339	Pa×s	583.01	Joback Method
dvisc	0.0002056	Pa×s	543.30	Joback Method
dvisc	0.0003380	Pa×s	503.60	Joback Method
dvisc	0.0006050	Pa×s	463.90	Joback Method
hfust	32.00	kJ/mol	416.20	NIST Webbook
hfust	35.33	kJ/mol	412.50	NIST Webbook
hsubt	123.00 ± 2.00	kJ/mol	366.50	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=C94757&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

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

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