Diclofop methyl

Other names:	(.+/-.)-Diclofop-methyl
	2-(4-(2,4-Dichlorophenoxy)phenoxy)-methyl-propionate
	2-(4-(2,4-Dichlorophenoxy)phenoxy)propanoic acid methyl ester
	Dichlorfop-methyl
	Dicloflop-methyl
	Diclofop, methyl ester
	HOE 23408
	Hoegrass
	Hoelon
	Hoelon 3EC
	Illoxan
	Iloxan
	Methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate
	Methyl diclofop
	Propanoic acid, 2-[4-(2,4-dichlorophenoxy)phenoxy]-, methyl ester
	Propionic acid, 2-(4-(2,4-dichlorophenoxy)phenoxy)-, methyl ester
	diclofop-methyl
Inchi:	InChI=1S/C16H14Cl2O4/c1-10(16(19)20-2)21-12-4-6-13(7-5-12)22-15-8-3-11(17)9-14(15
InchiKey:	BACHBFVBHLGWSL-UHFFFAOYSA-N
Formula:	C16H14Cl2O3
SMILES:	COC(=O)C(C)Oc1ccc(Oc2ccc(Cl)cc2Cl)cc1
Mol. weight [g/mol]:	325.19
CAS:	51338-27-3

Physical Properties

Property code	Value	Unit	Source
gf	-190.45	kJ/mol	Joback Method
hf	-480.92	kJ/mol	Joback Method
hfus	34.14	kJ/mol	Joback Method
hvap	80.11	kJ/mol	Joback Method
log10ws	-3.82		Aqueous Solubility Prediction Method
logp	4.726		Crippen Method
mcvol	232.440	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	2395.00		NIST Webbook
rinpol	2339.00		NIST Webbook

rinpol	2395.00		NIST Webbook
rinpol	2339.00		NIST Webbook
tb	829.33	K	Joback Method
tc	1067.40	K	Joback Method
tf	315.26 ± 0.20	K	NIST Webbook
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.47	J/mol×K	829.33	Joback Method
cpg	628.73	J/mol×K	869.01	Joback Method
cpg	639.72	J/mol×K	908.69	Joback Method
cpg	649.44	J/mol×K	948.36	Joback Method
cpg	657.91	J/mol×K	988.04	Joback Method
cpg	665.11	J/mol×K	1027.72	Joback Method
cpg	671.04	J/mol×K	1067.40	Joback Method
dvisc	0.0003732	Pa×s	521.94	Joback Method
dvisc	0.0002341	Pa×s	573.17	Joback Method
dvisc	0.0001585	Pa×s	624.40	Joback Method
dvisc	0.0001139	Pa×s	675.63	Joback Method
dvisc	0.0000857	Pa×s	726.87	Joback Method
dvisc	0.0000670	Pa×s	778.10	Joback Method
dvisc	0.0000540	Pa×s	829.33	Joback Method
hfust	27.08	kJ/mol	314.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51338273&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume