Fenoxaprop-ethyl

Other names:	Propanoic acid, 2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]-, ethyl ester
	Propanoic acid, 2-(4-((6-chloro-2-benzoxazolyl)oxy)phenoxy)-, ethyl ester, (.+/-.)-
	Fenoxaprop ethyl ester
	Whip
	Puma
	Furore
	Acclaim
	HOE 33171
	HOE-A 25-01
	Ethyl 2-[4-(6-chlorobenzoxazolyl-2-oxy)phenoxy]propionate
	ethyl 2-[4-[(6-chlorobenzoxazol-2-yl)oxy]phenoxy]propionate
Inchi:	InChI=1S/C18H16ClNO5/c1-2-22-17(21)9-10-23-13-4-6-14(7-5-13)24-18-20-15-8-3-12(1
InchiKey:	ZZJKDQVEAHXHLK-UHFFFAOYSA-N
Formula:	C18H16ClNO5
SMILES:	CCOC(=O)CCOc1ccc(Oc2nc3ccc(Cl)cc3o2)cc1
Mol. weight [g/mol]:	361.78
CAS:	116573-18-3

Physical Properties

Property code	Value	Unit	Source
chs	-8630.30 ± 5.00	kJ/mol	NIST Webbook
hfs	-762.80 ± 6.10	kJ/mol	NIST Webbook
log10ws	-9.75		Crippen Method
logp	4.606		Crippen Method
mcvol	249.070	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116573183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume