QUIZALOFOP--P-ETHYL

Other names: Propanoic acid, 2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]-, ethyl ester, (2R)-
Quizalofop-p
Quizalofop-p-ethyl Ethyl(R)-2-[4-(6-chloroquinoxalin-2-yloxy)]phenoxy]propionate
ethyl (R)-2-(4-((6-chloroquinoxalin-2-yl)oxy)phenoxy)propanoate
ethyl (R)-2-[4-(6-chloroquinoxalin-2-yloxy)phenoxy]propionate
quizalofop-p-ethyl

Inchi: InChI=1S/C19H17ClN2O4/c1-3-24-19(23)12(2)25-14-5-7-15(8-6-14)26-18-11-21-17-10-1

InchiKey: OSUHJPCHFDQAIT-UHFFFAOYSA-N

Formula: C19H17ClN2O4

SMILES: CCOC(=O)C(C)Oc1ccc(Oc2cnc3cc(Cl)ccc3n2)cc1

Mol. weight [g/mol]: 372.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.99		Cheméo Relay (1.0)
logp	4.406		Crippen Method
mcvol	262.970	ml/mol	McGowan Method
tf	378.58	K	Cheméo Relay (1.0)
tt	348.76	K	Binary Solid-Liquid Solubility Determination and Model Correlation of Quizalofop-p-ethyl in Different Pure Solvents

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Binary Solid-Liquid Solubility Determination and Model Correlation of Quizalofop-p-ethyl in Different Pure Solvents: https://www.doi.org/10.1021/acs.jced.8b01181

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100646513&Units=SI

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

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature