Carfentrazone ethyl

Other names:	Benzenepropanoic acid, «alpha», 2-dichloro-5-[4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]- Ethyl alpha, ethyl ester, 2-dichloro-5-[4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-4-fluorob
Inchi:	InChI=1S/C15H14Cl2F3N3O3/c1-3-26-13(24)10(17)4-8-5-12(11(18)6-9(8)16)23-15(25)2
InchiKey:	MLKCGVHIFJBRCD-UHFFFAOYSA-N
Formula:	C15H14Cl2F3N3O3
SMILES:	CCOC(=O)C(Cl)Cc1cc(-n2nc(C)n(C(F)F)c2=O)c(F)cc1Cl
Mol. weight [g/mol]:	412.19
CAS:	128639-02-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	3.243		Crippen Method
mcvol	252.030	ml/mol	McGowan Method
rinpol	2327.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C128639021&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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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