

# PYRAFLUFEN-ETHYL

**Other names:** Acetic acid,  
**Inchi:** 2-[2-chloro-5-[4-chloro-5-(difluoromethoxy)-1-methyl-1H-pyrazol-3-yl]-4-fluorophenoxy]-  
ethyl ester  
**InchiKey:** APTZNLHMIGJTEW-UHFFFAOYSA-N  
**Formula:** C<sub>15</sub>H<sub>13</sub>Cl<sub>2</sub>F<sub>3</sub>N<sub>2</sub>O<sub>4</sub>  
**SMILES:** CCOC(=O)COc1cc(-c2nn(C)c(OC(F)F)c2Cl)c(F)cc1Cl  
**Mol. weight [g/mol]:** 413.18  
**CAS:** 129630-19-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.00		Crippen Method
logp	4.076		Crippen Method
mcvol	247.920	ml/mol	McGowan Method
rinpol	2355.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C129630199&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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  
**rinpol:** Non-polar retention indices

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