

## Macroscopic Pka's

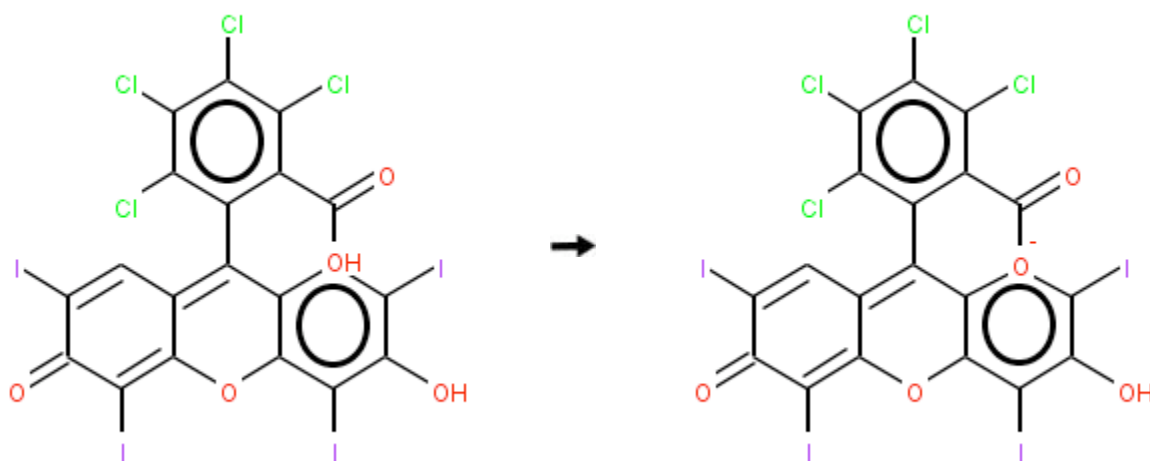
Smiles:

I-c(cc(c1OC2=C(I)C3=O)C(=C2C=C3I)-c(c(Cl)c(Cl)c4Cl)c(c4Cl)C(=O)O)c(O)c1I

The following macroscopic Pka estimates were generated from the crossing of the charge curves. All species curves of the same charge (as shown in the species plots) were summed and the crossing of these curves was taken as an estimate of the macroscopic Pka's.

Possible macroscopic constants are:

(1) For the reaction:

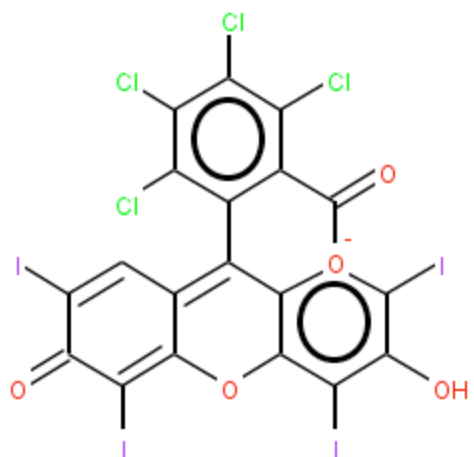


Max Fraction = 0.87

Max Fraction = 0.92

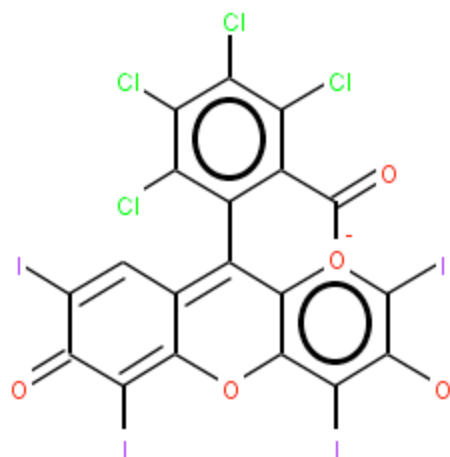
Macro Pka = 0.61

(2) For the reaction:



Max Fraction = 0.92

Macro Pka = 3.33



Max Fraction = 1.00