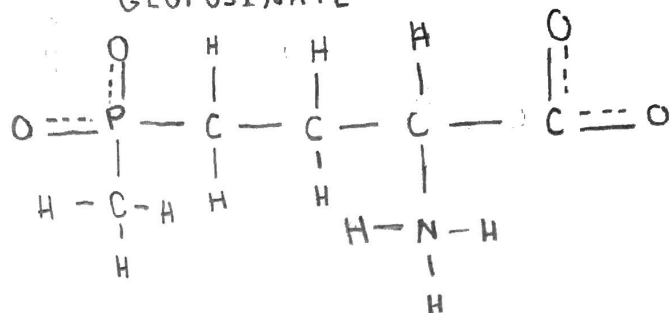
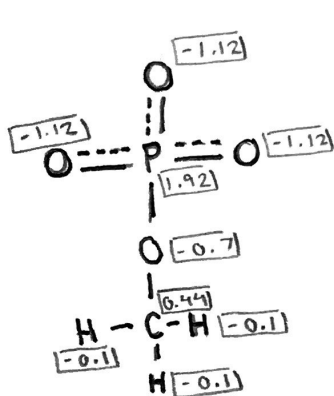


GLUFOSINATE



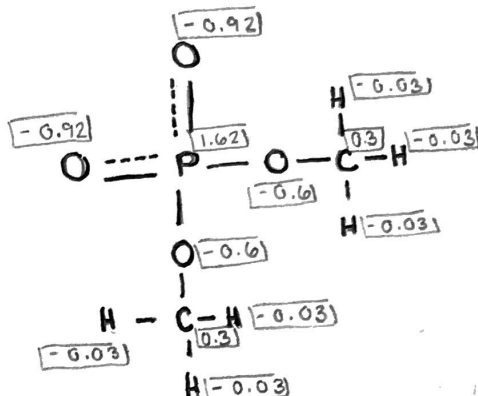
The OPLS database lists atom types for these 3 phosphorus-oxygen containing compounds:



METHYL PHOSPHATE

"Me Phosphate"

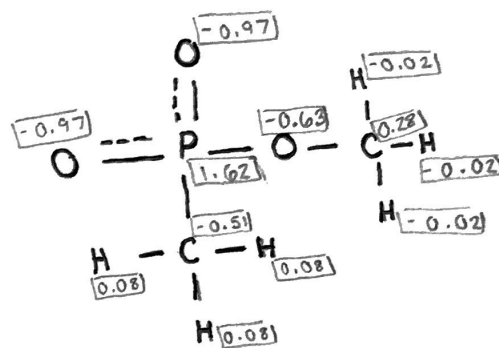
-2



DIMETHYL PHOSPHATE

"DiMe Phosphate"

-1



METHYL METHYLPHOSPHONATE

"Me Me Phosphonate"

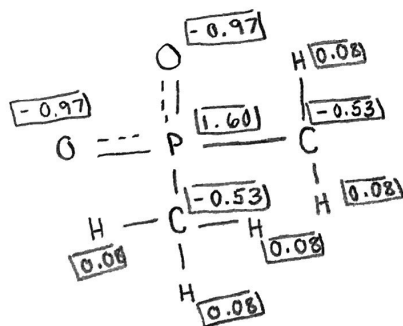
-1

No group is a perfect match for what is present in glufosinate.

The closest match appears to be methyl methylphosphonate, which has a methyl group directly attached to the central P.

If we treat the C in the alkane chain of glufosinate like the C in the methyl group of methyl methylphosphonate, we have the situation at left.

Distribute the remaining -0.06 evenly between the P and C atoms:



Charge: -1

Total Molecule:

