# Isofraxidin

**Inchi:** InChI=1S/C11H10O5/c1-14-7-5-6-3-4-8(12)16-10(6)11(15-2)9(7)13/h3-5,13H,1-2H3
**InchiKey:** HOEVRHHMDJKUMZ-UHFFFAOYSA-N
**Formula:** C11H10O5
**SMILES:** COc1cc2ccc(=O)oc2c(OC)c1O
**Mol. weight [g/mol]:** 222.19
**CAS:** 486-21-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -6.22 | | Crippen Method |
| logp | 1.516 | | Crippen Method |
| mcvol | 151.980 | ml/mol | McGowan Method |
| rinpol | 2085.00 | | NIST Webbook |

## Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C486215&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## 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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