

# Perillaketone

**Inchi:** InChI=1S/C10H14O2/c1-8(2)3-4-10(11)9-5-6-12-7-9/h5-8H,3-4H2,1-2H3  
**InchiKey:** LVHLZMUFIYAEQB-UHFFFAOYSA-N  
**Formula:** C10H14O2  
**SMILES:** CC(C)CCC(=O)c1ccoc1  
**Mol. weight [g/mol]:** 166.22  
**CAS:** 553-84-4

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.30   |        | Crippen Method |
| logp          | 2.898   |        | Crippen Method |
| mcvol         | 139.740 | ml/mol | McGowan Method |
| rinpol        | 1249.00 |        | NIST Webbook   |
| rinpol        | 1230.00 |        | NIST Webbook   |
| rinpol        | 1248.00 |        | NIST Webbook   |
| rinpol        | 1252.00 |        | NIST Webbook   |
| rinpol        | 1230.00 |        | NIST Webbook   |
| rinpol        | 1248.00 |        | NIST Webbook   |
| ripol         | 1811.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C553844&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**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  
**ripol:** Polar retention indices

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