

# 5-(2,4-dimethylheptanyl)-3-methyl-2H-pyran-2-one

**diastereomer 1**  
InChI: InChI=1S/C15H24O2/c1-5-6-11(2)9-12(3)10-14-8-7-13(4)15(16)17-14/h7-8,11-12H,5-6,9H  
InChIKey: PEMQRVSHWJTBLD-UHFFFAOYSA-N

**Formula:** C15H24O2  
**SMILES:** CCCC(C)CC(C)Cc1ccc(C)c(=O)o1  
**Mol. weight [g/mol]:** 236.35

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -8.35   |        | Crippen Method |
| logp          | 3.953   |        | Crippen Method |
| mcvol         | 210.190 | ml/mol | McGowan Method |
| rinpol        | 1806.00 |        | NIST Webbook   |
| rinpol        | 1806.00 |        | NIST Webbook   |
| ripol         | 2504.00 |        | NIST Webbook   |
| ripol         | 2504.00 |        | NIST Webbook   |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R494743&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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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