

# Poligodial + m-Tyr (ethyl ester) adduct (R,S)

**Inchi:** InChI=1S/C26H33NO3/c1-5-30-24(29)22(15-18-8-6-9-20(28)14-18)27-16-19-10-11-23-25  
**InchiKey:** RPYXDMDPPHKZFL-JGZAQREWSA-N  
**Formula:** C26H33NO3  
**SMILES:** CCOC(=O)C(Cc1cccc(O)c1)n1cc2c(c1)C1(C)CCCC(C)(C)C1C=C2  
**Mol. weight [g/mol]:** 407.55

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.51   |        | Crippen Method |
| logp          | 5.651   |        | Crippen Method |
| mcvol         | 331.250 | ml/mol | McGowan Method |
| rinpola       | 3005.00 |        | NIST Webbook   |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R163781&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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  
**rinpola:** Non-polar retention indices

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