# Bioresmethrin, isomer 2

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|---|---|
| **Inchi:** | InChI=1S/C22H26O3/c1-15(2)10-19-20(22(19,3)4)21(23)25-14-17-12-18(24-13-17)11-16 |
| **InchiKey:** | VEMKTZHHVJILDY-UHFFFAOYSA-N |
| **Formula:** | C22H26O3 |
| **SMILES:** | CC(C)=CC1C(C(=O)OCc2coc(Cc3ccccc3)c2)C1(C)C |
| **Mol. weight [g/mol]:** | 338.44 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -10.26 | | Crippen Method |
| logp | 5.152 | | Crippen Method |
| mcvol | 275.770 | ml/mol | McGowan Method |
| rinpol | 2413.00 | | NIST Webbook |
| rinpol | 2413.00 | | NIST Webbook |

## Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R566333&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

## Legend

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|---|---|
| **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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