

# Bioresmethrin, isomer 2

**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

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R566333&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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

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