

Bioresmethrin, isomer 1

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: VEMKTZHVVJILDY-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	2401.00		NIST Webbook
rinpol	2401.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R566328&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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