# Decursinol angelate

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|---|---|
| **Inchi:** | InChI=1S/C19H20O5/c1-5-11(2)18(21)23-16-9-13-8-12-6-7-17(20)22-14(12)10-15(13)24 |
| **InchiKey:** | AGABNGOXUSXQDD-YLBKJFSISA-N |
| **Formula:** | C19H20O5 |
| **SMILES:** | CC=C(C)C(=O)OC1Cc2cc3ccc(=O)oc3cc2OC1(C)C |
| **Mol. weight [g/mol]:** | 328.36 |
| **CAS:** | 130848-06-5 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -9.12 | | Crippen Method |
| logp | 3.384 | | Crippen Method |
| mcvol | 245.240 | ml/mol | McGowan Method |
| rinpol | 2757.00 | | NIST Webbook |
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| rinpol | 2757.00 | | NIST Webbook |

## Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C130848065&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

## 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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