# heraclenin

**Inchi:** InChI=1S/C16H14O5/c1-16(2)11(21-16)8-19-15-13-10(5-6-18-13)7-9-3-4-12(17)20-14(9)
**InchiKey:** CTJZWFCPUDPLME-NSHDSACASA-N
**Formula:** C16H14O5
**SMILES:** CC1(C)OC1COc1c2occc2cc2ccc(=O)oc12
**Mol. weight [g/mol]:** 286.28
**CAS:** 2880-49-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -12.97 | | Crippen Method |
| logp | 3.095 | | Crippen Method |
| mcvol | 196.410 | ml/mol | McGowan Method |
| rinpol | 2462.20 | | NIST Webbook |
| rinpol | 2456.00 | | NIST Webbook |
| rinpol | 2462.20 | | NIST Webbook |
| rinpol | 2456.00 | | NIST Webbook |

## Sources

**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=C2880491&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## 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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