

# 6-Iodocoumarin

**Inchi:** InChI=1S/C9H5IO2/c10-7-2-3-8-6(5-7)1-4-9(11)12-8/h1-5H  
**InchiKey:** JMTPGBQVDFBWFT-UHFFFAOYSA-N  
**Formula:** C9H5IO2  
**SMILES:** O=c1ccc2cc(I)ccc2o1  
**Mol. weight [g/mol]:** 272.04

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.58		Crippen Method
logp	2.398		Crippen Method
mcvol	132.010	ml/mol	McGowan Method
rinpol	1805.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1859.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R274267&Units=SI>

## 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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