

# 6-Cyanocoumarin

**Inchi:** InChI=1S/C10H5NO2/c11-6-7-1-3-9-8(5-7)2-4-10(12)13-9/h1-5H  
**InchiKey:** MCSNBULGQKALQK-UHFFFAOYSA-N  
**Formula:** C10H5NO2  
**SMILES:** N#Cc1ccc2oc(=O)ccc2c1  
**Mol. weight [g/mol]:** 171.15

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.78		Crippen Method
logp	1.665		Crippen Method
mcvol	121.660	ml/mol	McGowan Method
rinpol	1579.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1651.00		NIST Webbook

## Sources

**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=R274247&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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