

# Curzerenone

**Inchi:** InChI=1S/C15H20O2/c1-6-15(5)7-11-12(10(4)8-17-11)14(16)13(15)9(2)3/h8,13H,2,6-7H  
**InchiKey:** KTDQZLJOU MVWTK-UKRRQHHQSA-N  
**Formula:** C15H18O2  
**SMILES:** C=C(C)C1C(=O)c2c(C)coc2CC1(C)CC  
**Mol. weight [g/mol]:** 230.30  
**CAS:** 20493-56-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	3.935		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
rinpol	1574.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1595.50		NIST Webbook
rinpol	1609.60		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1610.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2240.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C20493565&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/57-923-4/Curzerenone.pdf>

Generated by Cheméo on 2024-06-30 23:21:40.201809207 +0000 UTC m=+22078949.122386580.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.