

# Graveoline

**Inchi:** InChI=1S/C17H13NO3/c1-18-13-5-3-2-4-12(13)15(19)9-14(18)11-6-7-16-17(8-11)21-10-  
**InchiKey:** COBBNRKBTCBWQP-UHFFFAOYSA-N  
**Formula:** C17H13NO3  
**SMILES:** Cn1c(-c2ccc3c(c2)OCO3)cc(=O)c2ccccc21  
**Mol. weight [g/mol]:** 279.29  
**CAS:** 485-61-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.80		Crippen Method
logp	2.934		Crippen Method
mcvol	200.140	ml/mol	McGowan Method
rinpola	3140.70		NIST Webbook
rinpola	3140.70		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C485610&Units=SI>  
**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)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpola:** Non-polar retention indices

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