

# Isooctylhydrocupreine

**Other names:** (8«alpha»,9R)-10,11-dihydro-6'-[(6-methylheptyl)oxy]cinchonan-9-ol  
**Inchi:** InChI=1S/C27H40N2O2/c1-4-20-18-29-14-12-21(20)16-26(29)27(30)23-11-13-28-25-10-  
**InchiKey:** DIOGDSVVUWNLHM-UHFFFAOYSA-N  
**Formula:** C27H40N2O2  
**SMILES:** CCC1CN2CCC1CC2C(O)c1ccnc2ccc(OCCCCC(C)C)cc12  
**Mol. weight [g/mol]:** 424.62  
**CAS:** 130-87-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.71		Crippen Method
logp	5.984		Crippen Method
mcvol	358.050	ml/mol	McGowan Method
rinpola	3103.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C130870&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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