

1H-Indole-3-ethanol, 2-(5-ethenyl-1-azabicyclo[2.2.2]oct-2-yl)-, [1S-(1«alpha»,2«alpha»,4«alpha»,5«beta»)]-

Other names:

Cinchonamine

InChI: InChI=1S/C19H24N2O/c1-2-13-12-21-9-7-14(13)11-18(21)19-16(8-10-22)15-5-3-4-6-17(

InchiKey: YAUKSCGKZYUZRH-UHFFFAOYSA-N

Formula: C19H24N2O

SMILES: C=CC1CN2CCC1CC2c1[nH]c2cccc2c1CCO

Mol. weight [g/mol]: 296.41

CAS: 482-28-0

Physical Properties

Property code	Value	Unit	Source
chs	-10864.00	kJ/mol	NIST Webbook
log10ws	-4.48		Crippen Method
logp	2.790		Crippen Method
mcvol	239.460	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: 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=C482280&Units=SI>

Legend

chs: Standard solid enthalpy of combustion

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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