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]c2ccccc2c1CCO
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/ci990307l
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