[2,2'-Bimorphinan]-3,3',6,6'-tetrol, 7,7',8,8'-tetradehydro-4,5:4',5'-diepoxy-17,17'-dime (5«alpha»,6«alpha»)-(5'«alpha»,6'«alpha»)-

Other names: Pseudomorphine
Inchi: InChI=1S/C34H36N2O6/c1-35-9-7-33-19-3-5-23(37)31(33)41-29-25(39)15(13-21(19)35)1
InchiKey: FOJYFDFNGPRXDR-UHFFFAOYSA-N
Formula: C34H36N2O6
SMILES: CN1CCC23c4c5cc(-c6cc7c8c(c6O)OC6C(O)C=CC9C(C7)N(C)CCC896)c(O)c4OC2C(O)
Mol. weight [g/mol]: 568.66
CAS: 125-24-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.71		Crippen Method
logp	2.377		Crippen Method
mcvol	402.100	ml/mol	McGowan Method
rinpol	2770.00		NIST Webbook
rinpol	2770.00		NIST Webbook

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=C125246&Units=SI

Legend

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

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