

N-Methyl-2,3-dihydroxymorphinan

Inchi: InChI=1S/C17H23NO2/c1-18-7-6-17-5-3-2-4-12(17)14(18)8-11-9-15(19)16(20)10-13(11)
InchiKey: SRBUIBKILLVEPZ-MRXJRLSOSA-N
Formula: C17H23NO2
SMILES: CN1CCC23CCCCC2C1Cc1cc(O)c(O)cc13
Mol. weight [g/mol]: 273.37

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.90 | | Crippen Method |
| logp | 2.786 | | Crippen Method |
| mcvol | 215.770 | ml/mol | McGowan Method |
| rinpol | 2500.00 | | NIST Webbook |
| rinpol | 2500.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R18165&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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