Methyldihydromorphine

Inchi: InChI=1S/C18H23NO3/c1-17(21)6-5-11-12-9-10-3-4-13(20)15-14(10)18(11,16(17)22-15)
InchiKey: NBKVWIJQJMEQLE-KDTAJPGPSA-N
Formula: C18H23NO3
SMILES: CN1CCC23c4c5ccc(O)c4OC2C(C)(O)CCC3C1C5
Mol. weight [g/mol]: 301.38
CAS: 509-56-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.86		Crippen Method
logp	1.812		Crippen Method
mcvol	224.870	ml/mol	McGowan Method
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C509568&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: 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
rinpol: Non-polar retention indices