

Metopon

Other names:

Morphinan-6-one, 4,5-«alpha»-epoxy-3-hydroxy-5,17-dimethyl-Dihydro-5-methylmorphinone
4,5-«alpha»-Epoxy-3-hydroxy-5,17-diethylmorphinan-6-one
Methyldihydromorphinone
5-Methyldihydromorphinone
Morphinone, dihydro-5-methyl-
Morphinone, methyldihydro-
(5«alpha»)-4,5-Epoxy-3-hydroxy-5,17-dimethylmorphinan-6-one
Morphinan-6-one, 4,5-epoxy-3-hydroxy-5,17-dimethyl-, (5«alpha»)-

Inchi: InChI=1S/C18H21NO3/c1-17-14(21)6-4-11-12-9-10-3-5-13(20)16(22-17)15(10)18(11,17)
InchiKey: NPZXCTIHHUUEEJ-UHFFFAOYSA-N
Formula: C18H21NO3
SMILES: CN1CCC23c4c5ccc(O)c4OC2(C)C(=O)CCC3C1C5
Mol. weight [g/mol]: 299.36
CAS: 143-52-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	2.020		Crippen Method
mcvol	220.570	ml/mol	McGowan Method
rinpol	2380.00		NIST Webbook
rinpol	2459.00		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=C143522&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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