Morphinan-6-ol, 4,5-epoxy-3-methoxy-17-methyl-, (5«alpha»,6«alpha»)-

Other names: (-)-Dihydrocodeine
3-Methoxy-12-methyl-5,6,7,7a,8,9-hexahydro-4aH-8,9c-iminoethanophenanthro(4,5-bcd)
4,5«alpha»-Epoxy-3-methoxy-17-methylmorphinan-6«alpha»-ol
4,5Â«alphaÂ»-Epoxy-3-methoxy-17-methylmorphinan-6Â«alphaÂ»-ol
6-Hydroxy-3-methoxy-N-methyl-4,5-epoxymorphinan
6«alpha»-Hydrocodol
6Â«alphaÂ»-Hydrocodol
7,8-Dihydrocodeine
8,14-Dihydroneopine
Codeine, 7,8-dihydro-
Codeine, dihydro-
Codhydrine
Cohydrin
DF 118
DH-codeine
Dehacodin
Didrate
Dihydrin
Dihydrocodeine
Dihydrocodeine Bitartrate
Dihydrokodein
Dihydroneopine
Drocode
Hydrocodeine
Hydrocodin
Morphinan-6«alpha»-ol, 4,5«alpha»-epoxy-3-methoxy-17-methyl-
Morphinan-6Â«alphaÂ»-ol, 4,5Â«alphaÂ»-epoxy-3-methoxy-17-methyl-
NSC 231319
Nadeine
Novcodin
Novicodin
Novicondin
Paracodin
Paracodine
Parzone
Rapacodin
Rapocodin
«alpha»-Hydrocodol
Â«alphaÂ»-Hydrocodol

Inchi: InChI=1S/C18H23NO3/c1-19-8-7-18-11-4-5-13(20)17(18)22-16-14(21-2)6-3-10(15(16)18

InchiKey: RBOXVHNMENFORY-UHFFFAOYSA-N
Formula: C18H23NO3
SMILES: COc1ccc2c3c1OC1C(O)CCC4C(C2)N(C)CCC341
Mol. weight [g/mol]: 301.38
CAS: 125-28-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.00		Aqueous Solubility Prediction Method
logp	1.725		Crippen Method
mcvol	224.870	ml/mol	McGowan Method
rinpol	2365.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2474.90		NIST Webbook
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
rinpol	2323.00		NIST Webbook
rinpol	2376.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2474.90		NIST Webbook
rinpol	2376.00		NIST Webbook
tf	385.65	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C125280&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
tf:	Normal melting (fusion) point