Acetyldihydrocodeine

Other names: (5«alpha»,6«alpha»)-4,5-epoxy-3-methoxy-17-methylmorphinan-6-yl acetate
(5Â«alphaÂ»,6Â«alphaÂ»)-4,5-epoxy-3-methoxy-17-methylmorphinan-6-yl acetate
7,8-Dihydrocodeine acetate
Acetylcodone
Acetyldihydrokodein
Codeine, acetyldihydro-
Codeine, dihydro-, acetate
Dihydrocodeine 6-acetate
Dihydrothebacone
Morphinan-6-ol, 4,5-epoxy-3-methoxy-17-methyl-, acetate (ester), (5 alpha, 6 alpha)-
Morphinan-6-ol, 4,5-epoxy-3-methoxy-17-methyl-, acetate (ester), (5«alpha» 6«alpha»)-
Morphinan-6-ol, 4,5-epoxy-3-methoxy-17-methyl-, acetate (ester), (5Â«alphaÂ» 6Â«alphaÂ»)-
Morphinan-6-ol, 4,5-epoxy-3-methoxy-17-methyl-, acetate, (5«alpha»,6«alpha»)-
Morphinan-6-ol, 4,5-epoxy-3-methoxy-17-methyl-, acetate, (5Â«alphaÂ»,6Â«alphaÂ»)-
Morphinan-6«alpha»-ol, 4,5-«alpha»-epoxy-3-methoxy-17-methyl-, acetate
Morphinan-6«alpha»-ol, 4,5«alpha»-epoxy-3-methoxy-17-methyl-, acetate (ester)
Morphinan-6Â«alphaÂ»-ol, 4,5-Â«alphaÂ»-epoxy-3-methoxy-17-methyl-, acetate
Morphinan-6Â«alphaÂ»-ol, 4,5Â«alphaÂ»-epoxy-3-methoxy-17-methyl-, acetate (ester)

Inchi: InChI=1S/C20H25NO4/c1-11(22)24-16-7-5-13-14-10-12-4-6-15(23-3)18-17(12)20(13,19(

InchiKey: LGGDXXJAGWBUSL-UHFFFAOYSA-N

Formula: C20H25NO4

SMILES: COc1ccc2c3c1OC1C(OC(C)=O)CCC4C(C2)N(C)CCC341

Mol. weight [g/mol]: 343.42

CAS: 3861-72-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Aqueous Solubility Prediction Method
logp	2.296		Crippen Method
mcvol	254.620	ml/mol	McGowan Method
rinpol	2480.00		NIST Webbook
rinpol	2455.00		NIST Webbook
rinpol	2455.00		NIST Webbook
rinpol	2455.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3861721&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