

# Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, acetate (ester), (5«alpha»,6«alpha»)-

Other names:

6-Acetylcodeine  
Acetylcodeine

Codeine, acetate

Codeine, acetate (ester)

Codeine, acetyl-

Codeinone, acetyldihydro-

Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, acetate (ester), (5.alpha.,6.alpha.)-

Morphinan-6-«alpha»-ol, 7,8-didehydro-4,5-«alpha»-epoxy-3-methoxy-17-methyl-, acetate

Morphinan-6-Â«alphaÂ»-ol,

7,8-didehydro-4,5-Â«alphaÂ»-epoxy-3-methoxy-17-methyl-, acetate

Morphinan-6«alpha»-ol, 7,8-didehydro-4,5«alpha»-epoxy-3-methoxy-17-methyl-, acetate (ester)

Morphinan-6A«alphaA»-ol,

7,8-didehydro-4,5A«alphaA»-epoxy-3-methoxy-17-methyl-, acetate (ester)

O-Acetylcodeine

**Inchi:**

InChI=1S/C20H23NO4/c1-11(22)24-16-7-5-13-14-10-12-4-6-15(23-3)18-17(12)20(13,19)

**InchiKey:**

MFXFQKMUCYHPFQ-UHFFFAOYSA-N

**Formula:**

C20H23NO4

**SMILES:**

COc1ccc2c3c1OC1C(OC(C)=O)C=CC4C(C2)N(C)CCC341

**Mol. weight [g/mol]:**

341.40

**CAS:**

6703-27-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Aqueous Solubility Prediction Method
logp	2.072		Crippen Method
mcvol	250.320	ml/mol	McGowan Method
rinpol	2505.00		NIST Webbook
rinpol	2484.00		NIST Webbook
rinpol	2510.00		NIST Webbook
rinpol	2503.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2502.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2483.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2484.00		NIST Webbook
rinpol	2530.00		NIST Webbook

rinpol	2510.00	NIST Webbook
rinpol	2535.00	NIST Webbook
rinpol	2530.00	NIST Webbook
rinpol	2480.00	NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6703271&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**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

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