

Thebacon

Other names:	Dihydrocodeinone enol acetate Morphinan-6-ol, 6,7-didehydro-4,5-epoxy-3-methoxy-17-methyl-, acetate (ester), (5«alpha»)- Morphinan-6-ol, 6,7-didehydro-4,5«alpha»-epoxy-3-methoxy-17-methyl-, acetate (ester) Acetyldihydrocodeinone Tebacon Thebacone Morphinan-6-ol, 6,7-didehydro-4,5-epoxy-3-methoxy-17-methyl-, acetate, (5«alpha»)- Acedicon Demethyldihydrothebaine, acetate Morphinan-6-ol, 6,7-didehydro-4,5«alpha»-epoxy-3-methoxy-17-methyl-,acetate Thebaine, demethyldihydro-, acetate Thebaine, demethyldihydro-, acetate (ester) Acedikon Acetyldihydrokodeinon 3-Methoxy-N-methyl-4,5-epoxymorphin-6-en-6-yl acetate Acetyldemethyldihydrothebaine Acetyldihydrochodeinone Demethyldihydrothebaine acetate (ester) Morphinan-6-ol, 6,7-didehydro-4,5-epoxy-3-methoxy-17-methyl-, 6-acetate, (5«alpha»)- NSC 117860
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:	RRJQTGHQFYTZOW-UHFFFAOYSA-N
Formula:	C20H23NO4
SMILES:	COc1ccc2c3c1OC1C(OC(C)=O)=CCC4C(C2)N(C)CCC314
Mol. weight [g/mol]:	341.40
CAS:	466-90-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.421		Crippen Method
mcvol	250.320	ml/mol	McGowan Method
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook
rinpol	2533.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C466900&Units=SI

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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