Nicocodine

Other names:	Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, 3-pyridinecarboxylate (ester), (5«alpha»,6«alpha»)- Morphinan-6«alpha»-ol, 7,8-didehydro-4,5«alpha»-epoxy-3-methoxy-17-methyl-, nicotinate (ester) Codeine nicotinate Lyopect RC 146 Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, 3-pyridinecarboxylate, (5«alpha»,6«alpha»)- Morphinan-6-«alpha»-ol, 7,8-didehydro-4,5-«alpha»-epoxy-3-methoxy-17-methyl-, nicotinate Nicotinic acid, ester with codeine Nicotinic acid, 7,8-didehydro-4,5-«alpha»-epoxy-3-methoxy-17-methylmorphinan-6-«alpha»-yl ester 6-Nicotinoylcodeine
Inchi:	InChI=1S/C24H24N2O4/c1-26-11-9-24-16-6-8-19(29-23(27)15-4-3-10-25-13-15)22(24)30
InchiKey:	RYBGRHAWFUVMST-UHFFFAOYSA-N
Formula:	C24H24N2O4
SMILES:	COc1ccc2c3c1OC1C(OC(=O)c4cccnc4)C=CC4C(C2)N(C)CCC341
Mol. weight [g/mol]:	404.46
CAS:	3688-66-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	2.761		Crippen Method
mcvol	292.900	ml/mol	McGowan Method
rinpol	3408.00		NIST Webbook
rinpol	3408.00		NIST Webbook

Sources

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=C3688662&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices