Protopine

Other names:	7,13a-Secoberbin-13a-one, 7-methyl-2,3:9,10-bis(methylenedioxy)-
	Biflorine
	Corydinine
	Fumarine
	Macleyine
	Bis[1,3]benzodioxolo[4,5-c:5',6'-g]azecin-13(5H)-one, 4,6,7,14-tetrahydro-5-methyl-
	Hypercorine
	Protopin
Inchi:	InChI=1S/C20H19NO5/c1-21-5-4-13-7-18-19(25-10-24-18)8-14(13)16(22)6-12-2-3-17-20
InchiKey:	GPTFURBXHJWNHR-UHFFFAOYSA-N
Formula:	C20H19NO5
SMILES:	CN1CCc2cc3c(cc2C(=O)Cc2ccc4c(c2C1)OCO4)OCO3
Mol. weight [g/mol]:	353.37
CAS:	130-86-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.73		Crippen Method
logp	2.557		Crippen Method
mcvol	247.590	ml/mol	McGowan Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C130869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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