Colchicine

Other names:	Acetamide, N-(5,6,7,9-tetrahydro-1,2,3,10-tetramethoxy-9-oxobenzo[a]heptalen-7-yl)-, (S)- Colchineos Colchisol Colcin Colsaloid Condylon NSC 757 7«alpha»-H-Colchicine Benzo(a)heptalen-9(5H)-one, 7-acetamido-6,7-dihydro-1,2,3,10-tetramethoxy- Colchicin Colchicina N-Acetyl trimethylcolchicinic acid methylether
Inchi:	Acetamide, N-((7S)-5,6,7,9-tetrahydro-1,2,3,10-tetramethoxy-9-oxobenzo(a)heptalen-7-yl)- InChI=1S/C22H25NO6/c1-12(24)23-16-8-6-13-10-19(27-3)21(28-4)22(29-5)20(13)14-7-9
InchiKey:	IAKHMKGGTNLKSZ-MRXNPFEDSA-N
Formula:	C22H25NO6
SMILES:	COc1cc2c(c(OC)c1OC)-c1ccc(OC)c(=O)cc1C(NC(C)=O)CC2
Mol. weight [g/mol]:	399.44
CAS:	64-86-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.32		Crippen Method
logp	2.872		Crippen Method
mcvol	299.060	ml/mol	McGowan Method
rinpol	3340.00		NIST Webbook
rinpol	3340.00		NIST Webbook
rinpol	3340.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64868&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

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