N-Acetylcolchinol methyl ether

Other names:	Acetamide, N-(6,7-dihydro-3,9,10,11-tetramethoxy-5H-dibenzo(a,c)cyclohepten-5-yl)-, (S)- Colchinol, N-acetyl-, methyl ether SKF 287
Inchi:	InChI=1S/C21H25NO5/c1-12(23)22-17-9-6-13-10-18(25-3)20(26-4)21(27-5)19(13)15-8-7
InchiKey:	FEPNCXXZWLXIHV-UHFFFAOYSA-N
Formula:	C21H25NO5
SMILES:	COc1ccc2c(c1)C(N=C(C)O)CCc1cc(OC)c(OC)c(OC)c1-2
Mol. weight [g/mol]:	371.43
CAS:	65967-01-3

Physical Properties

Property code	Value	Unit	Source
hf	-608.41	kJ/mol	Joback Method
hvap	100.49	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.352		Crippen Method
mcvol	283.400	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
tb	1028.28	K	Joback Method
tc	1263.43	K	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65967013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature