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(NC(C)=O)CCc1cc(OC)c(OC)c(OC)c1-2

Mol. weight [g/mol]: 371.43

Physical Properties

Property code	Value	Unit	Source
hfus	45.48	kJ/mol	Joback Method
logp	3.511		Crippen Method
mcvol	283.400	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.52	J/mol×K	963.58	Joback Method
cpg	927.72	J/mol×K	1001.93	Joback Method
cpg	939.39	J/mol×K	1040.29	Joback Method
cpg	949.55	J/mol×K	1078.64	Joback Method
cpg	958.19	J/mol×K	1116.99	Joback Method
cpg	965.32	J/mol×K	1155.35	Joback Method
cpg	970.96	J/mol×K	1193.70	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65967013&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume