1-Alpha-2-methyl-8-methoxy-6,7-methylenedioxy-

Inchi: InChI=1S/C22H23NO7/c1-23-8-7-11-9-14-20(29-10-28-14)21(27-4)15(11)17(23)18-12-5-

InchiKey: AKNNEGZIBPJZJG-UHFFFAOYSA-N

Formula: C22H23NO7

SMILES: COc1ccc2c(c1OC)C(=O)OC2C1c2c(cc3c(c2OC)OCO3)CCN1C

Mol. weight [g/mol]: 413.42

CAS: 10421-76-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.78		Crippen Method
logp	2.882		Crippen Method
mcvol	287.510	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10421768&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume