

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/ci9903071>
Crippen Method: https://www.cheméo.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

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