Protopine-M (demethylene-methyl-) isomer-1, AC

Inchi: InChI=1S/C22H23NO6/c1-13(24)29-22-17-11-23(2)7-6-15-9-20-21(28-12-27-20)10-16(15
InchiKey: CCUVDLJAJUVHEJ-UHFFFAOYSA-N
Formula: C22H23NO6
SMILES: COc1ccc2c(c1OC(C)=O)CN(C)CCc1cc3c(cc1C(=O)C2)OCO3
Mol. weight [g/mol]: 397.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.96		Crippen Method
logp	2.762		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R289051&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.