Poligodial + 3-methoxy-4,5-methylenedioxyamphetamine (R,S) adduct, #1

Inchi: InChI=1S/C26H35NO4/c1-16(11-17-12-20(29-5)23-21(13-17)30-15-31-23)27-14-19-18(2

InchiKey: OLCIVMRXJKIXKL-LEZKPSFTSA-N

Formula: C26H35NO4

SMILES: COc1cc(CC(C)N2C=C3C(=CCC4C(C)(C)CCCC34C)C2O)cc2c1OCO2

Mol. weight [g/mol]: 425.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.02		Crippen Method
logp	5.036		Crippen Method
mcvol	334.860	ml/mol	McGowan Method
rinpol	3008.00		NIST Webbook
rinpol	3008.00		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=R163761&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

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