

Poligodial + 3-methoxy-4,5-methylenedioxyamphetamine

(R,S) adduct, # 2
PubChem ID: 197777
InChI: 197777 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	3016.00		NIST Webbook
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Sources

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R163776&Units=SI>

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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