

7-(1H-Pyrrol-2-yloxymethyl)-2,3,5,8-tetrahydro-1H-

Inchi: InChI=1S/C12H16N2O2/c15-10-4-7-14-6-3-9(12(10)14)8-16-11-2-1-5-13-11/h1-3,5,10,12
InchiKey: WFNLVEYQLWMQRZ-UHFFFAOYSA-N
Formula: C12H16N2O2
SMILES: OC1CCN2CC=C(COc3ccc[nH]3)C12
Mol. weight [g/mol]: 220.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	0.287		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
rinpol	2130.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R577912&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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