3',4'-Methylenedioxy-a-pyrrolidinopropiophenone

Other names: 3',4'-Methylenedioxy-a-pyrrolidinopropiophenone
R,S-3',4'-methylenedioxy-«alpha»-pyrrolidinopropiophenone
Inchi: InChI=1S/C14H17NO3/c1-10(15-6-2-3-7-15)14(16)11-4-5-12-13(8-11)18-9-17-12/h4-5,8,
InchiKey: NIYQOTCYXGXMPI-UHFFFAOYSA-N
Formula: C14H17NO3
SMILES: CC(C(=O)c1ccc2c(c1)OCO2)N1CCCC1
Mol. weight [g/mol]: 247.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Cheméo Relay (1.0)
logp	2.082		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook
tb	607.87	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24698575&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

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