5-(Methylenedioxyphenyl)-2-pentenoyl pyrrolidide

Inchi: InChI=1S/C16H19NO3/c18-16(17-9-3-4-10-17)6-2-1-5-13-7-8-14-15(11-13)20-12-19-14/l

InchiKey: XZTCTKKANUDQCW-QHHAFSJGSA-N

Formula: C16H19NO3

SMILES: O=C(C=CCCc1ccc2c(c1)OCO2)N1CCCC1

Mol. weight [g/mol]: 273.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	2.526		Crippen Method
mcvol	209.810	ml/mol	McGowan Method
rinpol	2572.00		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=R546042&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