4'-Methyl-«alpha»-(2-oxopyrrolidino)hexanophene

Other names: R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone-M (oxo-)
Inchi: InChI=1S/C17H23NO2/c1-3-4-6-15(18-12-5-7-16(18)19)17(20)14-10-8-13(2)9-11-14/h8-
InchiKey: IGGGRUIUYLKKLE-UHFFFAOYSA-N
Formula: C17H23NO2
SMILES: CCCCC(C(=O)c1ccc(C)cc1)N1CCCC1=O
Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	3.359		Crippen Method
mcvol	228.890	ml/mol	McGowan Method
rinpol	2165.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U314303&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.