4'-Methyl-«alpha»-pyrrolidinohexanophenone

Other names: R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone
Inchi: InChI=1S/C17H25NO/c1-3-4-7-16(18-12-5-6-13-18)17(19)15-10-8-14(2)9-11-15/h8-11,16
InchiKey: YOSQVMGMENUCDX-UHFFFAOYSA-N
Formula: C17H25NO
SMILES: CCCCC(C(=O)c1ccc(C)cc1)N1CCCC1
Mol. weight [g/mol]: 259.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	3.832		Crippen Method
mcvol	227.320	ml/mol	McGowan Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		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=U314299&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

Latest version available from:
https://www.chemeo.com/cid/90-461-0/4-Methyl-alpha-pyrrolidinohexanophenone.pdf

Generated by Cheméo on 2024-04-17 01:46:28.850625394 +0000 UTC m=+15607637.771202705.

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