4-[2-(2-Oxo-pyrrolidin-1-yl)-propionyl]-benzoic acid ethyl ester

Inchi: InChI=1S/C16H19NO4/c1-3-21-16(20)13-8-6-12(7-9-13)15(19)11(2)17-10-4-5-14(17)18/h
InchiKey: XJFDSJZWASBPAY-UHFFFAOYSA-N
Formula: C16H19NO4
SMILES: CCOC(=O)c1ccc(C(=O)C(C)N2CCCC2=O)cc1
Mol. weight [g/mol]: 289.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	2.057		Crippen Method
mcvol	222.240	ml/mol	McGowan Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R284234&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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/120-732-5/4-2-2-Oxo-pyrrolidin-1-yl-propionyl-benzoic-acid-ethyl-ester.pdf
Generated by Cheméo on 2024-04-28 19:07:57.072608011 +0000 UTC m=+16620525.993185328.

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