

R,S-4'-Methoxy-«alpha»-pyrrolidinopropiophenone

Other names:

(desmethyl-), ethylated
Pyrrolidine, 1-(1-(4-methoxybenzoyl)ethyl)

Inchi: InChI=1S/C15H21NO2/c1-3-18-14-8-6-13(7-9-14)15(17)12(2)16-10-4-5-11-16/h6-9,12H,

InchiKey: DJKDTLFRWPMBBA-UHFFFAOYSA-N

Formula: C₁₅H₂₁NO₂

SMILES: CCOc1ccc(C(=O)C(C)N2CCCC2)cc1

Mol. weight [g/mol]: 247.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	2.752		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
rinpola	1955.00		NIST Webbook
rinpola	1955.00		NIST Webbook
rinpola	1955.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R290581&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

rinpola: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/123-583-8/R-S-4-Methoxy-alpha-pyrrolidinopropiophenone-M-desmethyl-ethylated.pdf>

Generated by Cheméo on 2024-04-29 10:14:43.44765023 +0000 UTC m=+16674932.368227542.

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