Pyrrolidine, 1-(m-methoxycinnamoyl)-

Other names:	1-(m-Methoxycinnamoyl)pyrrolidine
Inchi:	InChI=1S/C14H17NO2/c1-17-13-6-4-5-12(11-13)7-8-14(16)15-9-2-3-10-15/h4-8,11H,2-3
InchiKey:	LAPTWLCIZWFMJK-BQYQJAHWSA-N
Formula:	C14H17NO2
SMILES:	COc1cccc(C=CC(=O)N2CCCC2)c1
Mol. weight [g/mol]:	231.29
CAS:	29647-01-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	2.331		Crippen Method
mcvol	186.620	ml/mol	McGowan Method
rinpol	2364.10		NIST Webbook
rinpol	2364.10		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29647016&Units=SI

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/116-434-1/Pyrrolidine-1-m-methoxycinnamoyl.pdf

Generated by Cheméo on 2024-10-12 09:00:13.459778096 +0000 UTC m=+3304476.096747344.

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