1-(4-methoxybenzoyl)pyrrolidin-2-one

Other names: aniracetam
Inchi: InChI=1S/C12H13NO3/c1-16-10-6-4-9(5-7-10)12(15)13-8-2-3-11(13)14/h4-7H,2-3,8H2,1
InchiKey: ZXNRTKGTQJPIJK-UHFFFAOYSA-N
Formula: C12H13NO3
SMILES: COc1ccc(C(=O)N2CCCC2=O)cc1
Mol. weight [g/mol]: 219.24

Physical Properties

Property code	Value	Unit	Source
hf	-383.76	kJ/mol	Cheméo Relay (1.0)
hvap	83.10	kJ/mol	Cheméo Relay (1.0)
ie	8.58	eV	Cheméo Relay (1.0)
log10ws	-2.19		Cheméo Relay (1.0)
logp	1.458		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
tb	629.52	K	Cheméo Relay (1.0)
tf	356.47	K	Cheméo Relay (1.0)

Sources

Aniracetam Solubility in Pure and Binary Solvents: Effect of Molecular Interaction and Analysis of Crystallized Products: https://www.doi.org/10.1021/acs.jced.8b00023
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point