Pyrrolidine, 1-(4-methoxyphenyl)

Inchi: InChI=1S/C11H15NO/c1-13-11-6-4-10(5-7-11)12-8-2-3-9-12/h4-7H,2-3,8-9H2,1H3
InchiKey: VVGHYJTYYXOIGG-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: COc1ccc(N2CCCC2)cc1
Mol. weight [g/mol]: 177.24
CAS: 54660-04-7

Physical Properties

Property code	Value	Unit	Source
affp	961.20	kJ/mol	NIST Webbook
basg	930.40	kJ/mol	NIST Webbook
log10ws	-2.23		Crippen Method
logp	2.295		Crippen Method
mcvol	147.080	ml/mol	McGowan Method

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=C54660047&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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