Pyrrolidine, 1-(4-methylphenyl)

Inchi: InChI=1S/C11H15N/c1-10-4-6-11(7-5-10)12-8-2-3-9-12/h4-7H,2-3,8-9H2,1H3
InchiKey: STRWKFUEXQHMFW-UHFFFAOYSA-N
Formula: C11H15N
SMILES: Cc1ccc(N2CCCC2)cc1
Mol. weight [g/mol]: 161.24
CAS: 54104-82-4

Physical Properties

Property code	Value	Unit	Source
affp	910.20	kJ/mol	NIST Webbook
basg	879.40	kJ/mol	NIST Webbook
log10ws	-2.59		Crippen Method
logp	2.595		Crippen Method
mcvol	141.210	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54104824&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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