

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: STRWKFUEXQHMFV-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/ci9903071>
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

Latest version available from:

<https://www.cheméo.com/cid/23-147-3/Pyrrolidine-1-4-methylphenyl.pdf>

Generated by Cheméo on 2024-10-08 14:39:07.724844853 +0000 UTC m=+2979210.361814102.

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