

Pyrrolidine, 1-(4-chlorophenyl)

Inchi: InChI=1S/C10H12ClN/c11-9-3-5-10(6-4-9)12-7-1-2-8-12/h3-6H,1-2,7-8H2
InchiKey: DPQIAEJLCJLSJK-UHFFFAOYSA-N
Formula: C10H12ClN
SMILES: Clc1ccc(N2CCCC2)cc1
Mol. weight [g/mol]: 181.66
CAS: 4280-30-2

Physical Properties

Property code	Value	Unit	Source
affp	937.40	kJ/mol	NIST Webbook
basg	906.60	kJ/mol	NIST Webbook
log10ws	-2.80		Crippen Method
logp	2.940		Crippen Method
mcvol	139.360	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=C4280302&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

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