N-[4-Chloro-2-nitrophenyl]pyrrolidine

Other names: Pyrrolidine, 1-(4-chloro-2-nitrophenyl)
Inchi: InChI=1S/C10H11ClN2O2/c11-8-3-4-9(10(7-8)13(14)15)12-5-1-2-6-12/h3-4,7H,1-2,5-6H2
InchiKey: QATZMIJXHKOELL-UHFFFAOYSA-N
Formula: C10H11ClN2O2
SMILES: O=[N+]([O-])c1cc(Cl)ccc1N1CCCC1
Mol. weight [g/mol]: 226.66
CAS: 41173-36-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	2.848		Crippen Method
mcvol	156.780	ml/mol	McGowan Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook

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=C41173368&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from: