N-[2-Amino-4-(trifluoromethyl)phenyl]pyrrolidine

Inchi: InChI=1S/C11H13F3N2/c12-11(13,14)8-3-4-10(9(15)7-8)16-5-1-2-6-16/h3-4,7H,1-2,5-6,1
InchiKey: HPDFKXPVMXSXGE-UHFFFAOYSA-N
Formula: C11H13F3N2
SMILES: Nc1cc(C(F)(F)F)ccc1N1CCCC1
Mol. weight [g/mol]: 230.23
CAS: 133184-80-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	2.888		Crippen Method
mcvol	156.500	ml/mol	McGowan Method

Sources

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=C133184802&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume