

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

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