

N-(2-Amino-4-trifluoromethylphenyl)morpholine

Other names:	N-[2-Amino-4-(trifluoromethyl)phenyl]morpholin
Inchi:	InChI=1S/C11H13F3N2O/c12-11(13,14)8-1-2-10(9(15)7-8)16-3-5-17-6-4-16/h1-2,7H,3-6
InchiKey:	CNVOJNRNRNAOOP-UHFFFAOYSA-N
Formula:	C11H13F3N2O
SMILES:	<chem>Nc1cc(C(F)(F)F)ccc1N1CCOCC1</chem>
Mol. weight [g/mol]:	246.23
CAS:	784-57-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	2.124		Crippen Method
mcvol	162.370	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=C784576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/93-337-5/N-2-Amino-4-trifluoromethylphenyl-morpholine.pdf>

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