Piperazine, 1-[3-(trifluoromethyl)phenyl]-

Other names:	1-[3-(Trifluoromethyl)phenyl]piperazine
	TFMPP
	N-(«alpha»,«alpha»,«alpha»-trifluoro-3-tolyl)piperazine
Inchi:	InChI=1S/C11H13F3N2/c12-11(13,14)9-2-1-3-10(8-9)16-6-4-15-5-7-16/h1-3,8,15H,4-7H2
InchiKey:	KKIMDKMETPPURN-UHFFFAOYSA-N
Formula:	C11H13F3N2
SMILES:	FC(F)(F)c1cccc(N2CCNCC2)c1
Mol. weight [g/mol]:	230.23
CAS:	15532-75-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	2.115		Crippen Method
mcvol	156.500	ml/mol	McGowan Method
rinpol	1558.00		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=C15532759&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