

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

<b>Other names:</b>	1-[3-(Trifluoromethyl)phenyl]piperazine TFMPP N-(«alpha», «alpha», «alpha»-trifluoro-3-tolyl)piperazine
<b>Inchi:</b>	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
<b>InchiKey:</b>	KKIMDKMETPPURN-UHFFFAOYSA-N
<b>Formula:</b>	C11H13F3N2
<b>SMILES:</b>	FC(F)(F)c1cccc(N2CCNCC2)c1
<b>Mol. weight [g/mol]:</b>	230.23
<b>CAS:</b>	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
rropol	1558.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C15532759&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15532759&amp;Units=SI</a>

## Legend

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

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