

3-Methylindole, N-trifluoroacetyl-

Other names:	3-Methylindole, TFA
Inchi:	InChI=1S/C11H8F3NO/c1-7-6-15(10(16)11(12,13)14)9-5-3-2-4-8(7)9/h2-6H,1H3
InchiKey:	PEJJIQKHDNSFNO-UHFFFAOYSA-N
Formula:	C11H8F3NO
SMILES:	<chem>Cc1cn(C(=O)C(F)(F)F)c2ccccc12</chem>
Mol. weight [g/mol]:	227.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	3.152		Crippen Method
mcvol	143.790	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=U328363&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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/20-551-7/3-Methylindole-N-trifluoroacetyl.pdf>

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