

1-Methylcarbazole, N-trifluoroacetyl-

Other names:	1-Methylcarbazole, TFA
Inchi:	InChI=1S/C15H10F3NO/c1-9-5-4-7-11-10-6-2-3-8-12(10)19(13(9)11)14(20)15(16,17)18/
InchiKey:	DABPARXNVIIMTD-UHFFFAOYSA-N
Formula:	C15H10F3NO
SMILES:	Cc1cccc2c3ccccc3n(C(=O)C(F)(F)F)c12
Mol. weight [g/mol]:	277.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.34		Crippen Method
logp	4.305		Crippen Method
mcvol	180.690	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U328375&Units=SI

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/91-328-7/1-Methylcarbazole-N-trifluoroacetyl.pdf>

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