

1,2,3,4-Tetrahydrocarbazole, N-trifluoroacetyl-

Other names:	1,2,3,4-Tetrahydrocarbazole, TFA
Inchi:	InChI=1S/C14H12F3NO/c15-14(16,17)13(19)18-11-7-3-1-5-9(11)10-6-2-4-8-12(10)18/h1
InchiKey:	LSHAYCXEJHPSFZ-UHFFFAOYSA-N
Formula:	C14H12F3NO
SMILES:	O=C(n1c2c(c3ccccc31)CCCC2)C(F)(F)F
Mol. weight [g/mol]:	267.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Crippen Method
logp	3.723		Crippen Method
mcvol	175.200	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=U328373&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/113-257-1/1-2-3-4-Tetrahydrocarbazole-N-trifluoroacetyl.pdf>

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