

Dodecahydrocarbazole, N-trifluoroacetyl-

Other names:	Dodecahydrocarbazole, TFA
Inchi:	InChI=1S/C14H20F3NO/c15-14(16,17)13(19)18-11-7-3-1-5-9(11)10-6-2-4-8-12(10)18/h9
InchiKey:	OVNMPOUZIAOESQ-UHFFFAOYSA-N
Formula:	C14H20F3NO
SMILES:	O=C(N1C2CCCCC2C2CCCC21)C(F)(F)F
Mol. weight [g/mol]:	275.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	3.509		Crippen Method
mcvol	192.400	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=U328360&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/64-780-5/Dodecahydrocarbazole-N-trifluoroacetyl.pdf>

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