

trans-Decahydroquinoline, N-trifluoroacetyl-

Other names:	trans-Decahydroquinoline, TFA
Inchi:	InChI=1S/C11H16F3NO/c12-11(13,14)10(16)15-7-3-5-8-4-1-2-6-9(8)15/h8-9H,1-7H2
InchiKey:	MAWPTHSOUMYTBJ-UHFFFAOYSA-N
Formula:	C11H16F3NO
SMILES:	O=C(N1CCCC2CCCCC21)C(F)(F)F
Mol. weight [g/mol]:	235.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	2.730		Crippen Method
mcvol	160.990	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=U328359&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/22-176-2/trans-Decahydroquinoline-N-trifluoroacetyl.pdf>

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