

# 1,4-Dimethylcarbazole, N-trifluoroacetyl-

<b>Other names:</b>	1,4-Dimethylcarbazole, TFA
<b>Inchi:</b>	InChI=1S/C16H12F3NO/c1-9-7-8-10(2)14-13(9)11-5-3-4-6-12(11)20(14)15(21)16(17,18)
<b>InchiKey:</b>	QJWLXMZHLKOYFC-UHFFFAOYSA-N
<b>Formula:</b>	C16H12F3NO
<b>SMILES:</b>	<chem>Cc1ccc(C)c2c1c1cccc1n2C(=O)C(F)(F)F</chem>
<b>Mol. weight [g/mol]:</b>	291.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.81		Crippen Method
logp	4.614		Crippen Method
mcvol	194.780	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U328383&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U328383&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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