

1,8-Dimethylcarbazole, N-trifluoroacetyl-

Other names:	1,8-Dimethylcarbazole, TFA
Inchi:	InChI=1S/C16H12F3NO/c1-9-5-3-7-11-12-8-4-6-10(2)14(12)20(13(9)11)15(21)16(17,18)
InchiKey:	KUVUOVQLDXATDV-UHFFFAOYSA-N
Formula:	C16H12F3NO
SMILES:	<chem>Cc1cccc2c3cccc(C)c3n(C(=O)C(F)(F)F)c12</chem>
Mol. weight [g/mol]:	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U328376&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/115-393-8/1-8-Dimethylcarbazole-N-trifluoroacetyl.pdf>

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