

1,5-Dimethylcazbazole, N-trifluoroacetyl-

Other names:	1,5-Dimethylcarbazole, TFA
Inchi:	InChI=1S/C16H12F3NO/c1-9-5-4-8-12-13(9)11-7-3-6-10(2)14(11)20(12)15(21)16(17,18)
InchiKey:	DDCUUMXQPFISPG-UHFFFAOYSA-N
Formula:	C16H12F3NO
SMILES:	<chem>Cc1cccc2c1c1ccc(C)c1n2C(=O)C(F)(F)F</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=U328384&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/120-100-6/1-5-Dimethylcazbazole-N-trifluoroacetyl.pdf>

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