1,3-Dimethylcarbazole, N-trifluoroacetyl-

Other names: 1,3-Dimethylcarbazole, TFA
Inchi: InChI=1S/C16H12F3NO/c1-9-7-10(2)14-12(8-9)11-5-3-4-6-13(11)20(14)15(21)16(17,18)
InchiKey: QKBDAOAFNJRVHH-UHFFFAOYSA-N
Formula: C16H12F3NO
SMILES: Cc1cc(C)c2c(c1)c1ccccc1n2C(=O)C(F)(F)F
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

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=U328381&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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