

1,7-Dimethylcarbazole, n-trifluoroacetyl-

Other names: 1,7-Dimethylcarbazole, TFA.

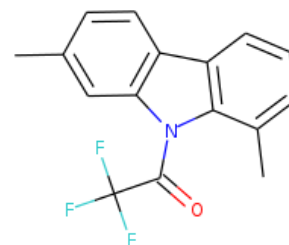
InChI: InChI=1S/C16H12F3NO/c1-9-6-7-11-12-5-3-4-10(2)14(12)20(13(11)8-9)15(21)16(17,18)19/h3-8H,1-2H3

InChI Key: GOGSOLVDVDADTC-UHFFFAOYSA-N

Formula: C16H12F3NO

SMILES: Cc1ccc2c3cccc(C)c3n(C(=O)C(F)(F)F)c2c1

Molecular Weight: 291.27



Physical Properties

| Property | Value | Unit | Source |
|---------------------------|-------|------|----------------|
| $\log P_{\text{oct/wat}}$ | 4.61 | | Crippen Method |

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H12F3NO/c1-9-6-7-11-12-5-3-4-10\(2\)14\(12\)20\(13\(11\)8-9\)15\(21\)16\(17,18\)19/h3-8H,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H12F3NO/c1-9-6-7-11-12-5-3-4-10(2)14(12)20(13(11)8-9)15(21)16(17,18)19/h3-8H,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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