

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: | QKBD AOAFNJR VHH-UHFFFAOYSA-N |
| Formula: | C16H12F3NO |
| SMILES: | <chem>Cc1cc(C)c2c(c1)c1cccc1n2C(=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

| | |
|------------------------|---|
| 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 |

Latest version available from:

<https://www.chemeo.com/cid/112-688-4/1-3-Dimethylcarbazole-N-trifluoroacetyl.pdf>

Generated by Cheméo on 2024-04-29 11:06:55.946188117 +0000 UTC m=+16678064.866765433.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.