

1-Methyl-2-trifluoro-methyl benzimidazole

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|-----------------------------|--|
| Inchi: | InChI=1S/C9H7F3N2/c1-14-7-5-3-2-4-6(7)13-8(14)9(10,11)12/h2-5H,1H3 |
| InchiKey: | YKKYRNSRLGCTDO-UHFFFAOYSA-N |
| Formula: | C9H7F3N2 |
| SMILES: | Cn1c(C(F)(F)F)nc2ccccc21 |
| Mol. weight [g/mol]: | 200.16 |
| CAS: | 384-46-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.43 | | Crippen Method |
| logp | 2.592 | | Crippen Method |
| mcvol | 124.020 | 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=C384463&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 |

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