

Pyridine, 3-(trifluoromethyl)-

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|-----------------------------|--|
| Other names: | 3-Trifluoromethylpyridine 3-(CF ₃)-Pyridine |
| Inchi: | InChI=1S/C6H4F3N/c7-6(8,9)5-2-1-3-10-4-5/h1-4H |
| InchiKey: | JTZSFNHHVULOGJ-UHFFFAOYSA-N |
| Formula: | C ₆ H ₄ F ₃ N |
| SMILES: | FC(F)(F)c1ccnc1 |
| Mol. weight [g/mol]: | 147.10 |
| CAS: | 3796-23-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| affp | 892.50 | kJ/mol | NIST Webbook |
| basg | 860.70 | kJ/mol | NIST Webbook |
| log10ws | -2.34 | | Crippen Method |
| logp | 2.100 | | Crippen Method |
| mcvol | 86.930 | 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=C3796234&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|-------------------------------------|
| affp: | Proton affinity |
| basg: | Gas basicity |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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