

# 5-Methylisoxazol-3-trifluoroacetylamine

**Inchi:** InChI=1S/C6H5F3N2O2/c1-3-2-4(11-13-3)10-5(12)6(7,8)9/h2H,1H3,(H,10,11,12)  
**InchiKey:** XHHJGKWYEHYLBC-UHFFFAOYSA-N  
**Formula:** C6H5F3N2O2  
**SMILES:** Cc1cc(=NC(=O)C(F)(F)F)[nH]o1  
**Mol. weight [g/mol]:** 194.11  
**CAS:** 211429-86-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	0.424		Crippen Method
mcvol	108.650	ml/mol	McGowan Method
rinpol	1081.00		NIST Webbook
rinpol	1081.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C211429866&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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