

# 1-Methyl-3-trifluoromethyl-2-pyrazolin-5-one

<b>Inchi:</b>	InChI=1S/C5H5F3N2O/c1-10-4(11)2-3(9-10)5(6,7)8/h2H2,1H3
<b>InchiKey:</b>	SYHYFYSGUQRNRS-UHFFFAOYSA-N
<b>Formula:</b>	C5H5F3N2O
<b>SMILES:</b>	CN1N=C(C(F)(F)F)CC1=O
<b>Mol. weight [g/mol]:</b>	166.10
<b>CAS:</b>	122431-37-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.97		Crippen Method
logp	0.767		Crippen Method
mcvol	92.990	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C122431372&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C122431372&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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