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

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C122431372&Units=SI

Legend

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