4,5-Dihydro-1H-pyrazole trifluoroacetate

Other names: 2-Pyrazoline trifluoroacetate
Inchi: InChI=1S/C5H5F3N2O/c6-5(7,8)4(11)10-3-1-2-9-10/h2H,1,3H2
InchiKey: VCHGCNMAXUBZQM-UHFFFAOYSA-N
Formula: C5H5F3N2O
SMILES: O=C(N1CCC=N1)C(F)(F)F
Mol. weight [g/mol]: 166.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.97		Crippen Method
logp	0.767		Crippen Method
mcvol	92.990	ml/mol	McGowan Method
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook

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=U372965&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
rinpol: Non-polar retention indices