2,3-Cyclohexenopyridine, 4-trifluoroacetyl

Inchi: InChI=1S/C11H10F3NO/c12-11(13,14)10(16)8-5-6-15-9-4-2-1-3-7(8)9/h5-6H,1-4H2
InchiKey: BZUCVQWONKKSDB-UHFFFAOYSA-N
Formula: C11H10F3NO
SMILES: O=C(c1ccnc2c1CCCC2)C(F)(F)F
Mol. weight [g/mol]: 229.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.06		Crippen Method
logp	2.705		Crippen Method
mcvol	148.090	ml/mol	McGowan Method
rinpol	178.42		NIST Webbook
rinpol	178.42		NIST Webbook

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=R598073&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.