3-(2-Pyridyl)propyl trifluoroacetate

Other names: 3-Pyridinepropanol, trifluoroacetate (ester)
Pyridine, 3-(3-trifluoroacetoxypropyl)-
Inchi: InChI=1S/C10H10F3NO2/c11-10(12,13)9(15)16-7-3-5-8-4-1-2-6-14-8/h1-2,4,6H,3,5,7H2
InchiKey: JMZGCPMOUHRDMC-UHFFFAOYSA-N
Formula: C10H10F3NO2
SMILES: O=C(OCCCc1ccccn1)C(F)(F)F
Mol. weight [g/mol]: 233.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	2.120		Crippen Method
mcvol	150.730	ml/mol	McGowan Method
rinpol	1230.00		NIST Webbook
rinpol	1230.00		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=U373168&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

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