2,3-Cyclopentenepyridine, 4-trifluoroacetyl

Inchi: InChI=1S/C10H8F3NO/c11-10(12,13)9(15)7-4-5-14-8-3-1-2-6(7)8/h4-5H,1-3H2
InchiKey: JFOHXOWJCUAYFI-UHFFFAOYSA-N
Formula: C10H8F3NO
SMILES: O=C(c1ccnc2c1CCC2)C(F)(F)F
Mol. weight [g/mol]: 215.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Crippen Method
logp	2.315		Crippen Method
mcvol	134.000	ml/mol	McGowan Method
rinpol	212.67		NIST Webbook
rinpol	212.67		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=R598088&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.