Isoquinoline, 1,2,3,4-tetrahydro-2-(trifluoroacetyl)-

Other names: 1,2,3,4-Tetrahydroisoquinoline, TFA
Ethanone, 1-(3,4-dihydro-2(1H)-isoquinolinyl)-2,2,2-trifluoro-
1,2,3,4-tetrahydro-2-trifluoroacetylisoquinoline

Inchi: InChI=1S/C11H10F3NO/c12-11(13,14)10(16)15-6-5-8-3-1-2-4-9(8)7-15/h1-4H,5-7H2

InchiKey: DVTYJMQWZHKOTG-UHFFFAOYSA-N

Formula: C11H10F3NO

SMILES: O=C(N1CCc2ccccc2C1)C(F)(F)F

Mol. weight [g/mol]: 229.20

CAS: 55649-51-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	2.134		Crippen Method
mcvol	148.090	ml/mol	McGowan Method

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=C55649519&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