

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

Other names:	1,2,3,4-Tetrahydroisoquinoline, TFA Ethanone, 1-(3,4-dihydro-2(1H)-isoquinoliny)-2,2,2-trifluoro-1,2,3,4-tetrahydro-2-trifluoroacetylisquinoline
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/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/122-705-3/Isoquinoline-1-2-3-4-tetrahydro-2-trifluoroacetyl.pdf>

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