Proline, N-(trifluoroacetyl)-

Other names:	L-Proline, N-trifluoroacetyl- 1-(Trifluoroacetyl)proline
Inchi:	InChI=1S/C7H8F3NO3/c8-7(9,10)6(14)11-3-1-2-4(11)5(12)13/h4H,1-3H2,(H,12,13)/t4-/m
InchiKey:	PHJVUZNDIHXSDI-SCSAIBSYSA-N
Formula:	C7H8F3NO3
SMILES:	O=C(O)C1CCCN1C(=O)C(F)(F)F
Mol. weight [g/mol]:	211.14
CAS:	134454-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.87		Crippen Method
logp	0.624		Crippen Method
mcvol	122.930	ml/mol	McGowan Method
rinpol	1374.80		NIST Webbook
rinpol	1374.80		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=C134454196&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