5-Methyl-9-azabicyclo[3.3.1]nonan-3-one, N-trifluoroacetyl

Inchi: InChI=1S/C11H14F3NO2/c1-10-4-2-3-7(5-8(16)6-10)15(10)9(17)11(12,13)14/h7H,2-6H2
InchiKey: RQXCMTBBUISLML-UHFFFAOYSA-N
Formula: C11H14F3NO2
SMILES: CC12CCCC(CC(=O)C1)N2C(=O)C(F)(F)F
Mol. weight [g/mol]: 249.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	2.051		Crippen Method
mcvol	162.560	ml/mol	McGowan Method
rinpol	1375.00		NIST Webbook
rinpol	1375.00		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=R577907&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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