Niacinamide, N-trifluoroacetyl-

Inchi: InChI=1S/C8H5F3N2O2/c9-8(10,11)7(15)13-6(14)5-2-1-3-12-4-5/h1-4H,(H,13,14,15)
InchiKey: JZQDJFHADPYCTI-UHFFFAOYSA-N
Formula: C8H5F3N2O2
SMILES: O=C(NC(=O)C(F)(F)F)c1cccnc1
Mol. weight [g/mol]: 218.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	0.900		Crippen Method
mcvol	128.230	ml/mol	McGowan Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		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=U374341&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

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