Niacinamide, N-pentafluoropropionyl-

Inchi: InChI=1S/C9H5F5N2O2/c10-8(11,9(12,13)14)7(18)16-6(17)5-2-1-3-15-4-5/h1-4H,(H,16,1
InchiKey: DWWFUMFEQPHDAK-UHFFFAOYSA-N
Formula: C9H5F5N2O2
SMILES: O=C(NC(=O)C(F)(F)C(F)(F)F)c1cccnc1
Mol. weight [g/mol]: 268.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	1.536		Crippen Method
mcvol	145.860	ml/mol	McGowan Method
rinpol	1808.00		NIST Webbook
rinpol	1808.00		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=U374342&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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