Niacinamide, N-heptafluorobutyryl-

Inchi: InChI=1S/C10H5F7N2O2/c11-8(12,9(13,14)10(15,16)17)7(21)19-6(20)5-2-1-3-18-4-5/h1
InchiKey: AQGBZAXSFMDMIA-UHFFFAOYSA-N
Formula: C10H5F7N2O2
SMILES: O=C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1cccnc1
Mol. weight [g/mol]: 318.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	2.171		Crippen Method
mcvol	163.490	ml/mol	McGowan Method
rinpol	1847.00		NIST Webbook
rinpol	1847.00		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=U374343&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.