Creatinine, 1-pentafluoropropionyl-

Inchi: InChI=1S/C7H6F5N3O2/c1-14-2-3(16)15(5(14)13)4(17)6(8,9)7(10,11)12/h13H,2H2,1H3
InchiKey: LJOCKFPXTVZKJS-UHFFFAOYSA-N
Formula: C7H6F5N3O2
SMILES: CN1CC(=O)N(C(=O)C(F)(F)C(F)(F)F)C1=N
Mol. weight [g/mol]: 259.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	0.419		Crippen Method
mcvol	136.260	ml/mol	McGowan Method
rinpol	2061.00		NIST Webbook
rinpol	2061.00		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=U374344&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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