Creatinine, N,N'-di(trifluoroacetyl)-

Inchi: InChI=1S/C8H5F6N3O3/c1-16-2-3(18)17(5(20)8(12,13)14)6(16)15-4(19)7(9,10)11/h2H2,
InchiKey: NLIXQAMYEPFSAT-UHFFFAOYSA-N
Formula: C8H5F6N3O3
SMILES: CN1CC(=O)N(C(=O)C(F)(F)F)C1=NC(=O)C(F)(F)F
Mol. weight [g/mol]: 305.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	0.294		Crippen Method
mcvol	153.690	ml/mol	McGowan Method
rinpol	1856.00		NIST Webbook
rinpol	1856.00		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=U374351&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.