Creatinine, 1-trifluoroacetyl-

Inchi: InChI=1S/C6H6F3N3O2/c1-11-2-3(13)12(5(11)10)4(14)6(7,8)9/h10H,2H2,1H3
InchiKey: ZHQHMMPGTLUUJT-UHFFFAOYSA-N
Formula: C6H6F3N3O2
SMILES: CN1CC(=O)N(C(=O)C(F)(F)F)C1=N
Mol. weight [g/mol]: 209.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	-0.216		Crippen Method
mcvol	118.630	ml/mol	McGowan Method
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374345&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.