Creatinine, 1-acetyl-

Inchi: InChI=1S/C6H9N3O2/c1-4(10)9-5(11)3-8(2)6(9)7/h7H,3H2,1-2H3
InchiKey: QMQDYPSDRZORPH-UHFFFAOYSA-N
Formula: C6H9N3O2
SMILES: CC(=O)N1C(=N)N(C)CC1=O
Mol. weight [g/mol]: 155.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.83		Crippen Method
logp	-0.758		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
rinpol	2041.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374346&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices