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

Inchi: InChI=1S/C8H11N3O3/c1-5(12)9-8-10(3)4-7(14)11(8)6(2)13/h4H2,1-3H3
InchiKey: VVYMPEHIEORSFO-UHFFFAOYSA-N
Formula: C8H11N3O3
SMILES: CC(=O)N=C1N(C)CC(=O)N1C(C)=O
Mol. weight [g/mol]: 197.19

Physical Properties

Property code	Value	Unit	Source
log10ws	0.31		Crippen Method
logp	-0.791		Crippen Method
mcvol	143.070	ml/mol	McGowan Method
rinpol	2215.00		NIST Webbook
rinpol	2215.00		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=U374348&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

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