

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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/69-098-8/Creatinine-1-acetyl.pdf>

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