

Creatinine

Other names:	1-Methylglyocyamidine 1-Methylhydantoin-2-imide 2-Imino-1,5-dihydro-1-methyl-4H-imidazol-4-one 2-imino-1-methylimidazolidin-4-one 4H-Imidazol-4-one, 2-amino-1,5-dihydro-1-methyl- 4H-Imidazol-4-one, 2-imino-1,5-dihydro-1-methyl-
Inchi:	InChI=1S/C4H7N3O/c1-7-2-3(8)6-4(7)5/h2H2,1H3,(H2,5,6,8)
InchiKey:	DDRJAANPRJIHGJ-UHFFFAOYSA-N
Formula:	C4H7N3O
SMILES:	CN1CC(=O)NC1=N
Mol. weight [g/mol]:	113.12
CAS:	60-27-5

Physical Properties

Property code	Value	Unit	Source
chs	-2334.53 ± 0.86	kJ/mol	NIST Webbook
chs	-2336.00 ± 0.42	kJ/mol	NIST Webbook
chs	-2359.80	kJ/mol	NIST Webbook
hfs	-239.93 ± 0.88	kJ/mol	NIST Webbook
hfs	-238.50 ± 0.50	kJ/mol	NIST Webbook
log10ws	-0.83		Crippen Method
logp	-1.017		Crippen Method
mcvol	83.570	ml/mol	McGowan Method
ss	167.40	J/molxK	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	138.10	J/molxK	296.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The organisation of water around creatine and creatinine molecules:	https://www.doi.org/10.1016/j.jct.2018.08.007
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions

Latest version available from:

<https://www.chemeo.com/cid/14-521-7/Creatinine.pdf>

Generated by Cheméo on 2024-04-23 08:21:45.730486086 +0000 UTC m=+16149754.651063411.

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