Creatine

Other names:	(«alpha»-Methylguanido)acetic acid 6020-87-7 (hydrate) Creatin Glycine, N-(aminoiminomethyl)-N-methyl- Kreatin Krebiozon Methylguanidoacetic acid N-(Aminoiminomethyl)-N-methyl-glycine N-Methyl-N-guanylglycine N-amidinosarcasine N-amidinosarcosine N-guanyl-N-methylglycine NSC 8752
Inchi:	InChI=1S/C4H9N3O2/c1-7(4(5)6)2-3(8)9/h2H2,1H3,(H3,5,6)(H,8,9)
InchiKey:	CVSVTCORWBXHQV-UHFFFAOYSA-N
Formula:	C4H9N3O2
SMILES:	CN(CC(=O)O)C(=N)N
Mol. weight [g/mol]:	131.13
CAS:	57-00-1

Physical Properties

Property code	Value	Unit	Source
chs	-2323.10 ± 0.84	kJ/mol	NIST Webbook
chs	-2325.50	kJ/mol	NIST Webbook
gf	97.89	kJ/mol	Joback Method
hf	-91.05	kJ/mol	Joback Method
hfs	-537.18 ± 0.88	kJ/mol	NIST Webbook
hvap	72.69	kJ/mol	Joback Method
log10ws	-0.51		Crippen Method
logp	-1.104		Crippen Method
mcvol	100.300	ml/mol	McGowan Method
ss	189.50	J/mol×K	NIST Webbook
tb	606.28	K	Joback Method
tf	430.10	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.05	J/mol×K	606.28	Joback Method
cpg	50.00	J/mol×K	100.12	Joback Method
cpg	50.00	J/mol×K	100.12	Joback Method
cpg	50.00	J/mol×K	100.12	Joback Method
cpg	50.00	J/mol×K	100.12	Joback Method
cpg	50.00	J/mol×K	100.12	Joback Method
cpg	50.00	J/mol×K	100.12	Joback Method
cps	184.50	J/mol×K	323.00	NIST Webbook
cps	171.10	J/mol×K	296.30	NIST Webbook

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization 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
tb:	Normal Boiling Point Temperature

tf: Normal melting (fusion) point

Latest version available from:

https://www.chemeo.com/cid/15-170-6/Creatine.pdf

Generated by Cheméo on 2024-10-12 08:54:27.719443314 +0000 UTC m=+3304130.356412569.

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