Cyanoacetylurea

Other names:	2-Cyanoacetylurea
	Acetamide, N-(aminocarbonyl)-2-cyano-
	Urea, (cyanoacetyl)-
	1-(2-Cyanoacetyl)urea
	N-carbamoyl-2-cyanoacetamide
Inchi:	InChI=1S/C4H5N3O2/c5-2-1-3(8)7-4(6)9/h1H2,(H3,6,7,8,9)
InchiKey:	QJGRPCPCQQPZLZ-UHFFFAOYSA-N
Formula:	C4H5N3O2
SMILES:	N#CCC(=O)NC(N)=O
Mol. weight [g/mol]:	127.10
CAS:	1448-98-2

Physical Properties

Property code	Value	Unit	Source
gf	13.98	kJ/mol	Joback Method
hf	-98.91	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	65.54	kJ/mol	Joback Method
log10ws	-0.52		Crippen Method
logp	-0.905		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	623.44	K	Joback Method
tc	847.02	K	Joback Method
tf	435.61	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.69	J/mol×K	623.44	Joback Method
cpg	215.76	J/mol×K	660.70	Joback Method
cpg	221.42	J/mol×K	697.97	Joback Method
cpg	226.66	J/mol×K	735.23	Joback Method

cpg	231.51	J/mol×K	772.50	Joback Method
cpg	235.97	J/mol×K	809.76	Joback Method
cpg	240.05	J/mol×K	847.02	Joback Method

Sources

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=C1448982&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume