

Cyanuric acid

Other names:	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione
	1,3,5-triazine-2,4,6-triol
	2,4,6-Triazinetrione
	2,4,6-Trihydroxy-1,3,5-triazine
	2,4,6-Trihydroxy-S-triazine
	2,4,6-Trihydroxytriazine
	2,4,6-Trioxohexahydro-1,3,5-triazine
	5-Azabarbituric acid
	Isocyanurate acid
	Isocyanuric acid
	Kyselina kyanurova
	NSC 6284
	Pseudocyanuric acid
	Tricarbimide
	s-2,4,6-Triazinetriol
	s-Triazine-2,4,6-trione
	s-Triazinetriol
	s-Triazinetrione
	s-triazine-2,4,6(1H,3H,5H)-trione
	s-triazine-2,4,6-triol
	sym-Triazinetriol
	tricyanic acid
	trihydroxycyanidine
Inchi:	InChI=1S/C3H3N3O3/c7-1-4-2(8)6-3(9)5-1/h(H3,4,5,6,7,8,9)
InchiKey:	ZFSLODLOARCGLH-UHFFFAOYSA-N
Formula:	C3H3N3O3
SMILES:	Oc1nc(O)nc(O)n1
Mol. weight [g/mol]:	129.07
CAS:	108-80-5

Physical Properties

Property code	Value	Unit	Source
chs	-905.80 ± 1.50	kJ/mol	NIST Webbook
chs	-949.00 ± 2.00	kJ/mol	NIST Webbook
hf	-564.10 ± 1.50	kJ/mol	NIST Webbook
hfs	-703.50 ± 1.50	kJ/mol	NIST Webbook

hfs	-660.00 ± 2.00	kJ/mol	NIST Webbook
hsub	133.00	kJ/mol	NIST Webbook
log10ws	0.59		Crippen Method
logp	-1.012		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
ss	142.20	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	130.00	J/mol×K	298.15	NIST Webbook
cps	133.63	J/mol×K	300.00	NIST Webbook
hsubt	139.50	kJ/mol	470.00	NIST Webbook
hsubt	131.00	kJ/mol	456.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Tripolycyanamide and Cyanuric Acid in Ethanediol, N,N-Dimethylformamide, and N,N-Dimethylacetamide from (301.07 to 363.35) K:	https://www.doi.org/10.1021/je0342015 http://link.springer.com/article/10.1007/BF02311772 http://webbook.nist.gov/cgi/cbook.cgi?ID=C108805&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

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