

Cyanuric chloride

Other names:	1,3,5-Trichloro-2,4,6-triazine
	1,3,5-Trichlorotriazine
	2,4,6-Trichlor-(1,3,5)triazine
	2,4,6-Trichloro-1,3,5-triazine
	2,4,6-Trichloro-s-triazine
	2,4,6-Trichloro-sym-triazine
	2,4,6-Trichlorotriazine
	Chlorotriazine
	Cyanur chloride
	Cyanuric acid chloride
	Cyanuric trichloride
	Cyanuryl chloride
	Kyanurchlorid
	NSC 3512
	Trichloro-s-triazine
	Trichlorocyanidine
	Tricyanogen chloride
	UN 2670
	s-Triazine trichloride
	s-Triazine, 2,4,6-trichloro-
	s-Trichlorotriazine
	sym-Trichlorotriazine
	syn-Trichlotriazin
Inchi:	InChI=1S/C3Cl3N3/c4-1-7-2(5)9-3(6)8-1
InchiKey:	MGNCLNQXLYJVJD-UHFFFAOYSA-N
Formula:	C3Cl3N3
SMILES:	Clc1nc(Cl)nc(Cl)n1
Mol. weight [g/mol]:	184.41
CAS:	108-77-0

Physical Properties

Property code	Value	Unit	Source
chs	-1345.90 ± 2.10	kJ/mol	NIST Webbook
hfs	94.30 ± 2.50	kJ/mol	NIST Webbook
hfs	91.60	kJ/mol	NIST Webbook
hvap	62.59	kJ/mol	Cheméo Relay (1.0)

logp	1.832		Crippen Method
mcvol	96.030	ml/mol	McGowan Method
rinpol	1051.00		NIST Webbook
rinpol	1051.00		NIST Webbook
tb	463.20	K	NIST Webbook
tf	418.87 ± 0.10	K	NIST Webbook
tf	418.90 ± 0.06	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	463.20	K	96.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108770&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1460.mol

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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