# 1,3,5-Triazine, 2,4,6-trichloro-

**Other names:** 1,3,5-Trichloro-2,4,6-triazine
1,3,5-Trichlorotriazine
2,4,6-TRICHLORO-1,3,5-TRIAZINE
2,4,6-TRICHLORO-S-TRIAZINE
2,4,6-Trichlor-(1,3,5)triazine
2,4,6-Trichloro-sym-triazine
2,4,6-Trichlorotriazine
CYANURIC TRICHLORIDE
Chlorotriazine
Cyanur chloride
Cyanuric acid chloride
Cyanuric chloride
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 | 91.60 | kJ/mol | NIST Webbook |
| hfs | 94.30 ± 2.50 | kJ/mol | NIST Webbook |

| | | | |
|---|---|---|---|
| log10ws | -2.82 | | Crippen Method |
| 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

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

# Legend

**chs:** Standard solid enthalpy of combustion
**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
**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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