

Cyclonite

Other names:	1,3,5-Triazacyclohexane 1,3,5-trinitro- 1,3,5-Triazine, hexahydro-1,3,5-trinitro- 1,3,5-triaza-1,3,5-trinitrocyclohexane 1,3,5-triazine, hexahydro-1,3,5-trinitro 1,3,5-trinitro-1,3,5-triazacyclohexane 1,3,5-trinitrohexahydro-1,3,5-triazine 1,3,5-trinitrohexahydro-s-triazine 1,3,5-trinitroperhydro-1,3,5-triazine CX 84A Cyclonit Cyklonit Esaidro-1,3,5-trinitro-1,3,5-triazina Geksogen Heksogen Hexahydro-1,3,5-trinitro-1,3,5-triazin Hexogeen Hexogen Hexogen (explosive) Hexogen 5W Hexolite NSC 312447 PBX(AF) 108 PBXW 108(E) PE 4 RDX T4 Trimethyleentrinitramine Trinitrocyclotrimethylene triamine UN 0072 cyclotrimethylenenitramine cyclotrimethylenetrinitramine hexahydro-1,3,5-trinitro-1,3,5-triazine hexahydro-1,3,5-trinitro-s-triazine perhydro-1,3,5-trinitro-1,3,5-triazine s-triazine, hexahydro-1,3,5-trinitro- sym-Trimethylenetrinitramine trimethylenetrinitramine
Inchi:	InChI=1S/C3H6N6O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H2
InchiKey:	XTFIVUDBNACUBN-UHFFFAOYSA-N
Formula:	C3H6N6O6

SMILES: O=[N+](O-)[N1CN([N+](=O)[O-])CN([N+](=O)[O-])C1
Mol. weight [g/mol]: 222.12
CAS: 121-82-4

Physical Properties

Property code	Value	Unit	Source
chs	-2104.60 ± 2.10	kJ/mol	NIST Webbook
chs	-2120.00 ± 5.00	kJ/mol	NIST Webbook
chs	-2100.00	kJ/mol	NIST Webbook
chs	-2092.00 ± 2.10	kJ/mol	NIST Webbook
hf	192.00	kJ/mol	NIST Webbook
hfs	66.50 ± 2.10	kJ/mol	NIST Webbook
hfs	61.50	kJ/mol	NIST Webbook
hfs	79.10 ± 5.00	kJ/mol	NIST Webbook
hsub	134.30	kJ/mol	NIST Webbook
hsub	112.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-1.39		Crippen Method
logp	-1.646		Crippen Method
mcvol	124.470	ml/mol	McGowan Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1914.76		NIST Webbook
rinpol	1914.09		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1859.01		NIST Webbook
rinpol	1891.47		NIST Webbook
rinpol	1870.00		NIST Webbook
tf	478.50 ± 0.50	K	NIST Webbook
tf	477.10	K	Melting Behavior and Heat of Fusion of Compounds that Undergo Simultaneous Melting and Decomposition: An investigation with HMX
tf	477.35	K	HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior
tt	478.95	K	Thermal behavior of 1,3,5-trinitroso-1,3,5-triazinane and its melt-castable mixtures with cyclic nitramines

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	248.90	J/mol×K	298.00	NIST Webbook
hfust	37.66	kJ/mol	478.20	NIST Webbook
hfust	35.65	kJ/mol	478.50	NIST Webbook
hfust	37.66	kJ/mol	478.20	NIST Webbook
hsubt	130.10	kJ/mol	350.00	NIST Webbook
hsubt	112.50 ± 0.80	kJ/mol	342.50	NIST Webbook
hvapt	84.40	kJ/mol	513.00	NIST Webbook
psub	4.00e-06	kPa	348.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.90e-05	kPa	358.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	2.10e-05	kPa	363.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

psub	3.30e-05	kPa	368.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	4.60e-05	kPa	373.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	7.30e-05	kPa	378.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.14e-04	kPa	383.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	9.00e-06	kPa	353.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C121824&Units=SI>

Solubility of
Cyclotrimethylenetrinitramine (RDX) in
Binary Solvent Mixtures:

<https://www.doi.org/10.1021/je7002463>

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Triacetone triperoxide
thermogravimetric study of vapor
pressure and enthalpy of fusion of
compounds that melt in the range:
Simultaneous Melting and
Decomposition: An investigation with
DSC of the thermal behavior of
1,3,5-trinitroso-1,3,5-triazinane and its
high pressure polymers.
Parametric Overview of pressure influence
on the thermal analysis of a melt cast
composition based on cis
-1,3,4,6-tetranitrooctahydroimidazo-[4,5
d]imidazole (BCHMX)/trinitrotoluene
(TNT) compared with traditional
compositions

<https://www.doi.org/10.1016/j.tca.2010.11.034>
<https://www.doi.org/10.1021/acs.jced.6b00769>
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>
<https://www.doi.org/10.1016/j.tca.2015.07.010>
<https://www.doi.org/10.1016/j.tca.2016.03.018>
<https://www.doi.org/10.1016/j.tca.2018.06.006>

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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