1,3,5-Triazine, hexahydro-1,3,5-trinitro-

Other names:
1,3,5-Triazacyclohexane 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
cyclonite
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

Physical Properties

Property code	Value	Unit	Source
chs	-2120.00 ± 5.00	kJ/mol	NIST Webbook
chs	-2104.60 ± 2.10	kJ/mol	NIST Webbook
chs	-2092.00 ± 2.10	kJ/mol	NIST Webbook
chs	-2100.00	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	112.00 ± 2.00	kJ/mol	NIST Webbook
hsub	134.30	kJ/mol	NIST Webbook
logp	-1.646		Crippen Method
mcvol	124.470	ml/mol	McGowan Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1891.47		NIST Webbook
rinpol	1859.01		NIST Webbook
rinpol	1914.76		NIST Webbook
rinpol	1914.09		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

tt	477.95	K	Thermo-analytical study of a melt cast composition based on cis -1,3,4,6-tetranitrooctahydroimidazo-[4,5 d]imidazole (BCHMX)/trinitrotoluene (TNT) compared with traditional compositions

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	37.66	kJ/mol	478.20	NIST Webbook
hfust	35.65	kJ/mol	478.50	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	9.00e-06	kPa	353.15	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	1.90e-05	kPa	358.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	4.00e-06	kPa	348.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

Sources

HP-DSC study of energetic materials. Part I. Overview of pressure influence on thermal behavior:	https://www.doi.org/10.1016/j.tca.2016.03.018
Thermo-analytical study 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.2018.06.006
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Chemeo Relay (1.0):	

Melting Behavior and Heat of Fusion of Compounds that Undergo Simultaneous Melting and Decomposition: An investigation with HMX:	https://www.doi.org/10.1021/acs.jced.6b00769
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal behavior of 1,3,5-trinitroso-1,3,5-triazinane and its melt-castable mixtures with cyclic nitramines:	https://www.doi.org/10.1016/j.tca.2015.07.010
Solubility of Cyclotrimethylenetrinitramine (RDX) in Binary Solvent Mixtures:	https://www.doi.org/10.1021/je7002463
Chemeo Relay (1.0 beta):	
Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2010.11.034
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121824&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
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
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