1,3,5,7-Tetrazocine, octahydro-1,3,5,7-tetranitro-

Other names: 1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane
1,3,5,7-Tetraza-1,3,5,7-tetranitrocyclooctane
HMX
HMX (cyclotetramethylene tetranitramine)
HW 4
LX 14-0
Octagen
Octahydro-1,3,5,7-Tetranitro-s-tetrazocine
Oktogen
Tetramethylenetetranitramine
cyclotetramethylene tetranitramine
octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine
octogen
«beta» Hmy

Inchi: InChI=1S/C4H8N8O8/c13-9(14)5-1-6(10(15)16)3-8(12(19)20)4-7(2-5)11(17)18/h1-4H2

InchiKey: UZGLIIJVICEWHF-UHFFFAOYSA-N

Formula: C4H8N8O8

SMILES: O=[N+]([O-])N1CN([N+](=O)[O-])CN([N+](=O)[O-])CN([N+](=O)[O-])C1

Mol. weight [g/mol]: 296.16

Physical Properties

Property code	Value	Unit	Source
chs	-2820.00 ± 2.80	kJ/mol	NIST Webbook
chs	-2792.00	kJ/mol	NIST Webbook
chs	-2774.00	kJ/mol	NIST Webbook
chs	-2748.00	kJ/mol	NIST Webbook
hf	258.86	kJ/mol	Cheméo Relay (1.0)
hfs	75.00	kJ/mol	NIST Webbook
hfs	103.00 ± 2.80	kJ/mol	NIST Webbook
hfs	74.90	kJ/mol	NIST Webbook
logp	-2.195		Crippen Method
mcvol	165.960	ml/mol	McGowan Method
tf	553.90	K	Melting Behavior and Heat of Fusion of Compounds that Undergo Simultaneous Melting and Decomposition: An investigation with HMX

tt	465.25	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	290.20	J/mol×K	298.00	NIST Webbook
hfust	69.87	kJ/mol	553.15	NIST Webbook
hsubt	161.90	kJ/mol	474.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubility Measurement and Correlation for e-2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane in Five Organic Solvents at Temperatures between 283.15 and 333.15 K and Different Chloroalkane + Ethyl Acetate Binary Solvents at Temperatures between 283.15 and 323.15 K: https://www.doi.org/10.1021/acs.jced.6b00664

Standard Enthalpy of Formation, Thermal Behavior, and Specific Heat Capacity of 2HNIW*HMX Co-crystals: https://www.doi.org/10.1021/acs.jced.8b00454

Solubilities of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine in Butyrolactone + Water, Dimethyl Sulfoxide + Water, and N-Methyl-pyrrolidone + Water: https://www.doi.org/10.1021/je400199m

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2691410&Units=SI

Chemeo Relay (1.0, beta):

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

Cheméo Relay (1.0):

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

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

hsubt: Enthalpy of sublimation at a given temperature

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature