Cyclotetramethylenetetranitramine

Other names:	1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane
	1,3,5,7-Tetraza-1,3,5,7-tetranitrocyclooctane
	1,3,5,7-Tetrazocine, octahydro-1,3,5,7-tetranitro-
	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
CAS:	2691-41-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
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

Sources

Solubility Measurement and Correlation for	https://www.doi.org/10.1021/acs.jced.6b00664
Melting Behavior and Heat of Fusion of	https://www.doi.org/10.1021/acs.jced.6b00769
Compounds that Undergo	
Solubilities of Melting and	https://www.doi.org/10.1021/je400199m
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	http://link.springer.com/article/10.1007/BF02311772
Binary Aqueous Mixtures + Water	
Dimethylsulfoxide + Water and	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2691410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature