1,3,6-TRIAZACYCLOHEPTANE 1,3,6-TRINITRO-

Other names: 1,3,6-Triazacycloheptane 1,3,6-trinitro-
1,3,5-Trinitro-1,3,5-triazacycloheptane

Inchi: InChI=1S/C4H8N6O6/c11-8(12)5-1-2-6(9(13)14)4-7(3-5)10(15)16/h1-4H2

InchiKey: PWEBVDKVPUYMMO-UHFFFAOYSA-N

Formula: C4H8N6O6

SMILES: O=[N+]([O-])N1CCN([N+](=O)[O-])CN([N+](=O)[O-])C1

Mol. weight [g/mol]: 236.14

Physical Properties

Property code	Value	Unit	Source
hf	174.37	kJ/mol	Cheméo Relay (1.0)
logp	-1.604		Crippen Method
mcvol	138.560	ml/mol	McGowan Method
tf	461.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	27.74	kJ/mol	435.90	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5790783&Units=SI

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

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

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

Cheméo Relay (1.0):

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point