N,N',N''-Trinitro-1,3,5-triazacycloheptane

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
CAS:	5790-78-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.32		Crippen Method
logp	-1.604		Crippen Method
mcvol	138.560	ml/mol	McGowan Method

Temperature Dependent Properties

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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5790783&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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