1,1,3,5-Tetranitrohexahydropyrimidine

Other names: 1,3,5,5-Tetranitrohexahydropyrimidine
Inchi: InChI=1S/C4H6N6O8/c11-7(12)4(8(13)14)1-5(9(15)16)3-6(2-4)10(17)18/h1-3H2
InchiKey: NOEKJIBAIMWJEB-UHFFFAOYSA-N
Formula: C4H6N6O8
SMILES: O=[N+]([O-])N1CN([N+](=O)[O-])CC([N+](=O)[O-])([N+](=O)[O-])C1
Mol. weight [g/mol]: 266.13
CAS: 81360-42-1

Physical Properties

Property code	Value	Unit	Source
hfs	0.40	kJ/mol	NIST Webbook
log10ws	-1.95		Crippen Method
logp	-1.805		Crippen Method
mcvol	146.000	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.37	kJ/mol	430.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C81360421&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hfs:	Solid phase enthalpy of formation at standard conditions
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