1,3-Dinitro-1,3-diazacyclohexane

Inchi: InChI=1S/C4H8N4O4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H2
InchiKey: UMQHAPFYPBXHAF-UHFFFAOYSA-N
Formula: C4H8N4O4
SMILES: O=[N+]([O-])N1CCCN([N+](=O)[O-])C1
Mol. weight [g/mol]: 176.13
CAS: 5754-89-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.18		Crippen Method
logp	-0.665		Crippen Method
mcvol	111.160	ml/mol	McGowan Method
tf	354.00 ± 0.10	K	NIST Webbook
tf	353.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	2.97	kJ/mol	354.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5754892&Units=SI

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
tf:	Normal melting (fusion) point