1,4-Dinitro-1,4-diazacyclohexane

Other names:	N,N-Dinitropiperazine
	N,N'-Dinitropiperazine
	1,4-Dinitropiperazine
	1,4-Dinitro-1,4-diazacyclohexane
Inchi:	InChI=1S/C4H8N4O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h1-4H2
InchiKey:	GSUMZAMXDRIYCL-UHFFFAOYSA-N
Formula:	C4H8N4O4
SMILES:	O=[N+]([O-])N1CCN([N+](=O)[O-])CC1
Mol. weight [g/mol]:	176.13

Physical Properties

Property code	Value	Unit	Source
chs	-2664.00 ± 2.00	kJ/mol	NIST Webbook
hf	58.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-53.00 ± 2.00	kJ/mol	NIST Webbook
hsub	111.00 ± 0.80	kJ/mol	NIST Webbook
logp	-1.013		Crippen Method
mcvol	111.160	ml/mol	McGowan Method
tf	426.79	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	200.80	kJ/mol	489.20	NIST Webbook
hfust	33.93	kJ/mol	489.60	NIST Webbook
hsubt	111.00 ± 8.00	kJ/mol	342.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4164378&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):	
Cheméo Relay (1.0, beta):	

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point