1,3-DIAZACYCLOPENTAN-2-ONE 1,3-DINITRO-

Other names:	1,3-Dinitro-2-imidazolidone
	2-Imidazolidinone, 1,3-dinitro-
	N,N'-Dinitro-N,N'-ethyleneurea
	1,3-Diazacyclopentan-2-one 1,3-dinitro-
Inchi:	InChI=1S/C3H4N4O5/c8-3-4(6(9)10)1-2-5(3)7(11)12/h1-2H2
InchiKey:	XIWMHAHUHIHAER-UHFFFAOYSA-N
Formula:	C3H4N4O5
SMILES:	O=C1N([N+](=O)[O-])CCN1[N+](=O)[O-]
Mol. weight [g/mol]:	176.09

Physical Properties

Property code	Value	Unit	Source
chs	-1615.00	kJ/mol	NIST Webbook
hf	-38.64	kJ/mol	Cheméo Relay (1.0)
logp	-0.893		Crippen Method
mcvol	98.640	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2536187&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
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume