1-NITROSO-3,5-DINITRO-HEXAHYDRO-1,3,5-TRIA

Other names: 1,3-Dinitro-5-nitroso-1,3,5-triazacyclohexane
Inchi: InChI=1S/C3H6N6O5/c10-4-5-1-6(8(11)12)3-7(2-5)9(13)14/h1-3H2
InchiKey: LOSVOOKTCVILPF-UHFFFAOYSA-N
Formula: C3H6N6O5
SMILES: O=NN1CN([N+](=O)[O-])CN([N+](=O)[O-])C1
Mol. weight [g/mol]: 206.12

Physical Properties

Property code	Value	Unit	Source
hf	283.19	kJ/mol	Cheméo Relay (1.0)
logp	-1.157		Crippen Method
mcvol	118.600	ml/mol	McGowan Method
tf	455.08	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	25.97	kJ/mol	446.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5755271&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point