

1-Nitroso-3,5-dinitro-hexahydro-1,3,5-triazine

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
CAS:	5755-27-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	-1.157		Crippen Method
mccvol	118.600	ml/mol	McGowan Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5755271&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

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