

1,3,5,7-Tetraazabicyclo[3.3.1]nonane, 3,7-dinitroso-

Other names:

1,5-Methylene-3,7-dinitroso-1,3,5,7-tetraazacyclooctane
1,5-endo-Methylene-3,7-dinitroso-1,3,5,7-tetraazacyclooctane
3,7-Di-N-nitrosopentamethylenetetramine
3,7-dinitroso-1,3,5,7-tetraazabicyclo[3.3.1]nonane
Aceto DNPT 100
Aceto DNPT 40
Aceto DNPT 80
CHKHZ 18
Cellmic A 80
Chempor N 90
Chempor PC 65
DNMPT
DNPT
Di-N-Nitrosopentamethylenetetramine
Diasalt Bordeaux GP
Dinitrosopentamethenetetramine
Dinitrosopentamethylenetetraamine
Dinitrosopentamethylenetetramine
Dipentax
Dnpmt
Khempor N 90
Micropor
Mikrofor N
N,N'-Dinitrosopentamethylenetetramine
N,N-Dinitrosopentamethylenetetramine
N1,N3-Dinitrosopentamethylenetetramine
NSC 73599
Opex
Opex 93
Pentamethylenetetramine, dinitroso-
Porofor ChKhZ-18
Porofor DNO/F
Porofor chkhc-18
Porophor B
Unicel 100
Unicel NDX
Unicel-ND
Vulcacer B-40
Vulcacer BN
Vulcacer BN 94

Inchi: InChI=1S/C5H10N6O2/c12-6-10-2-8-1-9(4-10)5-11(3-8)7-13/h1-5H2
InchiKey: MWRWFPQBGSZWNV-UHFFFAOYSA-N
Formula: C5H10N6O2
SMILES: O=NN1CN2CN(C1)CN(N=O)C2
Mol. weight [g/mol]: 186.17
CAS: 101-25-7

Physical Properties

Property code	Value	Unit	Source
chs	-3624.90 ± 3.60	kJ/mol	NIST Webbook
chs	-3620.00	kJ/mol	NIST Webbook
hfs	228.20 ± 3.60	kJ/mol	NIST Webbook
hfs	185.60	kJ/mol	NIST Webbook
log10ws	-0.83		Crippen Method
logp	-0.628		Crippen Method
mcvol	122.610	ml/mol	McGowan Method

Sources

Solubility of 3,7-Dinitro-1,3,5,7-tetraazabicyclo[3.3.1]nonane in Ethanenitrile, Methanol, 1,1-Dichloroethane, Dimethyl Sulfoxide, Acetone, and Mixed Solvents: <https://www.doi.org/10.1021/acs.jced.5b00033>
 McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
 NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C101257&Units=SI>
 Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307i>
 Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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