Nitramine, N,N-bis(2-hydroxyethyl)-, nitrate

Other names:	2,2'-(Nitroimino)ethanol dinitrate
	2,2'-Dinitrato-N-nitrodiethylamine
	2,2'-Nitroiminobis(ethylnitrate)
	2,2'-Nitroiminodiethanol nitrate
	DINA
	DINA (explosive)
	Diethanol-N-nitramine dinitrate
	Diethanolnitramine dinitrate
	Ethanol, 2,2'-(nitroimino)bis-, dinitrate
	Ethanol, 2,2'-(nitroimino)bis-, dinitrate (ester)
	Ethanol, 2,2'-nitroiminodi-, dinitrate
	N-Nitrodiethanolamine dinitrate
	Nitrodiethanolamine dinitrate
	sym-Dinitroxydiethylnitramine
Inchi:	InChI=1S/C4H8N4O8/c9-6(10)5(1-3-15-7(11)12)2-4-16-8(13)14/h1-4H2
InchiKey:	NZDNCDGEHXHPCO-UHFFFAOYSA-N
Formula:	C4H8N4O8
SMILES:	O=[N+]([O-])OCCN(CCO[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	240.13

Physical Properties

Property code	Value	Unit	Source
chl	-2459.90	kJ/mol	NIST Webbook
chs	-2409.90	kJ/mol	NIST Webbook
chs	-2407.00	kJ/mol	NIST Webbook
chs	-2410.60 ± 1.50	kJ/mol	NIST Webbook
chs	-2400.00	kJ/mol	NIST Webbook
hf	-155.17	kJ/mol	Cheméo Relay (1.0)
hfl	-257.42	kJ/mol	NIST Webbook
hfl	-224.00	kJ/mol	NIST Webbook
hfl	-224.00	kJ/mol	NIST Webbook
hfs	-306.80 ± 1.50	kJ/mol	NIST Webbook
hfs	-311.00	kJ/mol	NIST Webbook
hfs	-307.50	kJ/mol	NIST Webbook
hfus	45.60	kJ/mol	Joback Method
hvap	91.40	kJ/mol	Cheméo Relay (1.0)
ie	10.73	eV	Cheméo Relay (1.0)

log10ws	-2.08		Cheméo Relay (1.0)
logp	-1.103		Crippen Method
mcvol	141.200	ml/mol	McGowan Method
tb	523.03	K	Cheméo Relay (1.0)
tf	324.63	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.87	J/mol×K	803.72	Joback Method
cpg	416.08	J/mol×K	844.63	Joback Method
cpg	423.42	J/mol×K	885.54	Joback Method
cpg	429.90	J/mol×K	926.45	Joback Method
cpg	435.53	J/mol×K	967.36	Joback Method
cpg	440.31	J/mol×K	1008.27	Joback Method
cpg	444.27	J/mol×K	1049.18	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4185471&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

Legend

chl: Standard liquid enthalpy of combustion

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point