1,4-Cyclohexanedicarboxamide, n,n'-bis(2-chloroethyl)-n,n'-dinitroso-, trans-

Inchi: InChI=1S/C12H18Cl2N4O4/c13-5-7-17(15-21)11(19)9-1-2-10(4-3-9)12(20)18(16-22)8-6-14/h9-10H,1-8H2/t9-,10-

InchiKey: VXIKYYMERMEAJF-UHFFFAOYSA-N

Formula: C12H18Cl2N4O4

SMILES: O=NN(CCCl)C(=O)C1CCC(C(=O)N(CCCl)N=O)CC1

Mol. weight [g/mol]: 353.20

CAS: 13860-70-3

Physical Properties

Property code	Value	Unit	Source
hf	-714.99	kJ/mol	Joback Method
hvap	86.97	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.290		Crippen Method
mcvol	239.760	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
tb	823.12	K	Joback Method
tc	1029.73	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13860703&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature