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

Inchi: InChI=1S/C10H16Cl2N6O4/c11-1-3-17(13-21)9(19)15-5-7-16(8-6-15)10(20)18(14-22)4-2

InchiKey: CFKCAGGJBVJIHJ-UHFFFAOYSA-N

Formula: C10H16Cl2N6O4

SMILES: O=NN(CCCl)C(=O)N1CCN(C(=O)N(CCCl)N=O)CC1

Mol. weight [g/mol]: 355.18

CAS: 13907-80-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	1.288		Crippen Method
mcvol	231.540	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13907807&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume