

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(CCCI)C(=O)N1CCN(C(=O)N(CCCI)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

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