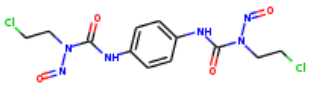
Urea, 1,1'-p-phenylenebis[3-(2-chloroethyl)-3-nitroso-

InChI: InChI=1S/C12H14Cl2N6O4/c13-5-7-19(17-23)11(21)15-9-1-2-10(4-3-9)16-12(22)20(18-24)8-6-14/h1-4H,5-8H2,(H,15,21)(H,16,22)
InChI Key: PCLGVSQVYVGFSH-UHFFFAOYSA-N
Formula: C12H14Cl2N6O4
SMILES: O=NN(CCCl)C(=O)Nc1ccc(NC(=O)N(CCCl)N=O)cc1
Molecular Weight: 377.18
CAS: 13907-59-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f H°_{gas}$	-416.97	kJ/mol	Joback Method
$\Delta_{vap} H°$	102.66	kJ/mol	Joback Method
$logP_{oct/wat}$	3.19		Crippen Method
P_c	2460.47	kPa	Joback Method
T_{boil}	940.24	K	Joback Method
T_c	1159.34	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14Cl2N6O4/c13-5-7-19(17-23)11(21)15-9-1-2-10(4-3-9)16-12(22)20(18-24)8-6-14/h1-4H,5-8H2,(H,15,21)(H,16,22)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$logP_{oct/wat}$: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).

T_c: Critical Temperature (K).