

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)

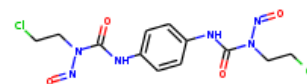
InChI Key: PCLGVSQVYVGFSSH-UHFFFAOYSA-N

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
$\Delta_f H^\circ_{\text{gas}}$	-416.97	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	102.66	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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,\(H,15,21\)\(H,16,22\)](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/ci9903071>

Legend

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

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