

Urea, 1-(2-chloroethyl)-1-nitroso-3-phenyl-

InChI: InChI=1S/C9H10ClN3O2/c10-6-7-13(12-15)9(14)11-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,11,14)

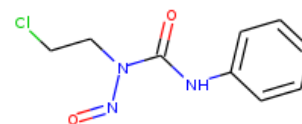
InChI Key: NTFJBCLCDARIRQ-UHFFFAOYSA-N

Formula: C₉H₁₀ClN₃O₂

SMILES: O=NN(CCCl)C(=O)Nc1ccccc1

Molecular Weight: 227.65

CAS: 13206-67-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f H^\circ_{\text{gas}}$	-168.07	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	66.61	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.44		Crippen Method
P_c	3333.53	kPa	Joback Method
T_{boil}	649.31	K	Joback Method
T_c	863.52	K	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H10ClN3O2/c10-6-7-13\(12-15\)9\(14\)11-8-4-2-1-3-5-8/h1-5H,6-7H2,\(H,11,14\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H10ClN3O2/c10-6-7-13(12-15)9(14)11-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,11,14))

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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