

# Benzamide, 2,5-dichloro-n-cyanomethyl-3-nitro-

**InChI:** InChI=1S/C9H5Cl2N3O3/c10-5-3-6(9(15)13-2-1-12)8(11)7(4-5)14(16)17/h3-4H,2H2,(H,13,15)

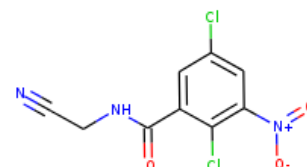
**InChI Key:** SCHAPWDTKXLDEP-UHFFFAOYSA-N

**Formula:** C9H5Cl2N3O3

**SMILES:** N#CCNC(=O)c1cc(Cl)cc([N+](=O)[O-])c1Cl

**Molecular Weight:** 274.06

**CAS:** 22978-18-3



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	213.76	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	36.56	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	39.90	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	88.91	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.155		Crippen Method
$P_c$	3062.55	kPa	Joback Method
$T_{\text{boil}}$	879.76	K	Joback Method
$T_c$	1137.44	K	Joback Method
$T_{\text{fus}}$	626.20	K	Joback Method
$V_c$	0.678	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	405.46	J/mol×K	879.76	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H5Cl2N3O3/c10-5-3-6\(9\(15\)13-2-1-12\)8\(11\)7\(4-5\)14\(16\)17/h3-4H,2H2,\(H,13,15\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H5Cl2N3O3/c10-5-3-6(9(15)13-2-1-12)8(11)7(4-5)14(16)17/h3-4H,2H2,(H,13,15))

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

## Legend

$C_{p, gas}$ : Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

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

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

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

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

$P_c$ : Critical Pressure (kPa).

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

$T_c$ : Critical Temperature (K).

$T_{fus}$ : Normal melting (fusion) point (K).

$V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

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