4'-Bromo-2'-nitroacetanilide

Other names: 4-Bromo-2-nitroacetanilide; Acetamide, N-(4-bromo-2-nitrophenyl)-.

InChI: InChI=1S/C8H7BrN2O3/c1-5(12)10-7-3-2-6(9)4-8(7)11(13)14/h2-4H,1H3,(H,10,12)

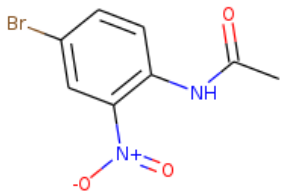
InChI Key: GUBNCRISSRANNO-UHFFFAOYSA-N

Formula: C8H7BrN2O3

SMILES: CC(=O)Nc1ccc(Br)cc1[N+](=O)[O-]

Molecular Weight: 259.06

CAS: 881-50-5



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	119.97	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-38.40	kJ/mol	Joback Method
$\Delta_{fus} H°$	33.08	kJ/mol	Joback Method
$\Delta_{vap} H°$	73.21	kJ/mol	Joback Method
$logP_{oct/wat}$	2.32		Crippen Method
P_c	4283.05	kPa	Joback Method
T_{boil}	741.12	K	Joback Method
T_c	1000.96	K	Joback Method
T_{fus}	537.38	K	Joback Method
V_c	0.56	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	345.90	J/mol×K	741.12	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H7BrN2O3/c1-5(12)10-7-3-2-6(9)4-8(7)11(13)14/h2-4H,1H3,(H,10,12)

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).