

## 2-(Acetyloxy)-5-bromobenzoic acid

**InChI:** InChI=1S/C9H7BrO4/c1-5(11)14-8-3-2-6(10)4-7(8)9(12)13/h2-4H,1H3,(H,12,13)

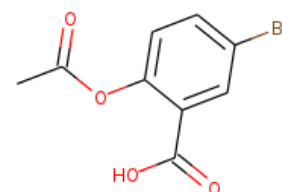
**InChI Key:** VRJBEVQGJOSGOX-UHFFFAOYSA-N

**Formula:** C9H7BrO4

**SMILES:** CC(=O)Oc1ccc(Br)cc1C(=O)O

**Molecular Weight:** 259.05

**CAS:** 1503-53-3



### Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-367.29	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-498.78	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	26.09	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	78.24	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.07		Crippen Method
$P_c$	4379.97	kPa	Joback Method
$T_{\text{boil}}$	730.46	K	Joback Method
$T_c$	951.00	K	Joback Method
$T_{\text{fus}}$	485.36	K	Joback Method
$V_c$	0.54	m <sup>3</sup> /kg-mol	Joback Method

### Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	339.38	J/mol×K	730.46	Joback Method
$\eta$	0.00	Paxs	730.46	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/C9H7BrO4/c1-5\(11\)14-8-3-2-6\(10\)4-7\(8\)9\(12\)13/h2-4H,1H3,\(H,12,13\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H7BrO4/c1-5(11)14-8-3-2-6(10)4-7(8)9(12)13/h2-4H,1H3,(H,12,13))

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

$\eta$ : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$ : 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).

$logP_{oct/wat}$ : 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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