

# 2-Acetamino-5-bromobenzoic acid

<b>Other names:</b>	N-Acetyl-5-bromo-anthranilic acid 2-Acetamido-5-bromobenzoic acid Benzoic acid, 2-(acetylamino)-5-bromo- 2-Acetylamino-5-bromobenzoic acid
<b>Inchi:</b>	InChI=1S/C9H8BrNO3/c1-5(12)11-8-3-2-6(10)4-7(8)9(13)14/h2-4H,1H3,(H,11,12)(H,13,14)
<b>InchiKey:</b>	QVABAFHRLMDDLML-UHFFFAOYSA-N
<b>Formula:</b>	C9H8BrNO3
<b>SMILES:</b>	CC(=O)Nc1ccc(Br)cc1C(=O)O
<b>Mol. weight [g/mol]:</b>	258.07
<b>CAS:</b>	38985-79-4

## Physical Properties

Property code	Value	Unit	Source
gf	-172.90	kJ/mol	Joback Method
hf	-313.09	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	82.27	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.106		Crippen Method
mcvol	150.400	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	758.21	K	Joback Method
tc	980.18	K	Joback Method
tf	515.79	K	Joback Method
vc	0.559	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.01	J/molxK	758.21	Joback Method
cpg	368.75	J/molxK	795.20	Joback Method
cpg	375.90	J/molxK	832.20	Joback Method
cpg	382.48	J/molxK	869.19	Joback Method
cpg	388.53	J/molxK	906.19	Joback Method

cpg	394.08	J/mol×K	943.18	Joback Method
cpg	399.17	J/mol×K	980.18	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C38985794&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38985794&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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