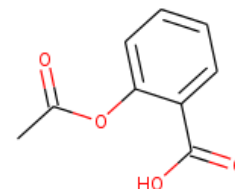


## Benzoic acid, 2-(acetyloxy)-

**Other names:** 2-(Acetyloxy)benzoic acid; 2-Acetoxybenzoic acid; 2-Acetylsalicylic acid; 2-Carboxyphenyl acetate; A.S.A.; A.S.A. Empirin; AC 5230; ASA; Acenterine; Acesal; Acesan; Acetal; Acetard; Aceticyl; Acetilsalicilico; Acetilum Acidulatum; Acetisal; Acetol; Acetonyl; Acetophen; Acetosal; Acetosalic acid; Acetosalin; Acetylin; Acetylsal; Acetylsalicylic acid; Acetylsalicylsaure; Acide acetylsalicylique; Acido O-acetil-benzoico; Acido acetilsalicilico; Acidum acetylsalicylicum; Acimetten; Acisal; Acylpyrin; Adiro; Asagran; Asatard; Ascoden-30; Ascolong; Aspalon; Aspec; Aspergum; Aspidrops; Aspirine; Aspro; Asropharm; Asteric; Bayer; Benaspir; Benzoic acid, 2-(acetyloxy)-; Bi-prin; Bialpirina; Bialpirinia; Bufferin; Caprin; Cemirit; Claradin; Clariprin; Colfarit; Colsprin; Contrheuma retard; Coricidin; Crystar; Decaten; Delgesic; Dolean PH 8; Duramax; ECM; Easprin; Ecolen; Ecotrin; Empirin; Endydol; Entericin; Enterophen; Enterosarein; Enterosarine; Entrophen; Extren; Globentyl; Globoid; Helicon; Idragin; Kapsazal; Kyselina 2-acetoxybenzoova; Kyselina acetylsalicylova; Levius; Magnecyl; Measurin; Micristin; Miniasal; Neuronika; Novid; Nu-seals; Nu-seals aspirin; O-acetylsalicylic acid; Persistin; Pharmacin; Pirseal; Polopiryna; Premaspin; Rheumintabletten; Rhodine; Rhonal; S-211; SP 189; Salacetin; Salcetogen; Saletin; Salicylic acid acetate.



**InChI:** InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)

**InChI Key:** BSYNRYMUTXBXSQ-UHFFFAOYSA-N

**Formula:** C9H8O4

**SMILES:** CC(=O)Oc1ccccc1C(=O)O

**Molecular Weight:** 180.16

**CAS:** 50-78-2

### Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-371.98	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-513.64	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	21.19	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	71.15	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.31		Crippen Method
$P_c$	4082.92	kPa	Joback Method
$T_{\text{boil}}$	659.32	K	Joback Method
$T_c$	868.49	K	Joback Method

Property	Value	Unit	Source
$T_{\text{fus}}$	409.00 ± 3.00	K	NIST Webbook
$T_{\text{fus}}$	414.00 ± 4.00	K	NIST Webbook
$T_{\text{fus}}$	405.00 ± 12.00	K	NIST Webbook
$T_{\text{fus}}$	412.00 ± 5.00	K	NIST Webbook
$T_{\text{fus}}$	403.00 ± 8.00	K	NIST Webbook
$T_{\text{fus}}$	415.00 ± 3.00	K	NIST Webbook
$T_{\text{fus}}$	414.00 ± 5.00	K	NIST Webbook
$T_{\text{fus}}$	410.00 ± 6.00	K	NIST Webbook
$T_{\text{fus}}$	410.00 ± 5.00	K	NIST Webbook
$T_{\text{fus}}$	402.00 ± 10.00	K	NIST Webbook
$T_{\text{fus}}$	405.00 ± 10.00	K	NIST Webbook
$T_{\text{fus}}$	388.00 ± 15.00	K	NIST Webbook
$T_{\text{fus}}$	388.00 ± 15.00	K	NIST Webbook
$T_{\text{fus}}$	387.00 ± 15.00	K	NIST Webbook
$T_{\text{fus}}$	409.80 ± 4.00	K	NIST Webbook
$T_{\text{fus}}$	408.00 ± 5.00	K	NIST Webbook
$T_{\text{fus}}$	406.00 ± 5.00	K	NIST Webbook
$T_{\text{fus}}$	402.00 ± 6.00	K	NIST Webbook
$T_{\text{fus}}$	401.00 ± 6.00	K	NIST Webbook
$T_{\text{fus}}$	396.00 ± 8.00	K	NIST Webbook
$T_{\text{fus}}$	387.00 ± 8.00	K	NIST Webbook
$T_{\text{fus}}$	397.00 ± 8.00	K	NIST Webbook
$T_{\text{fus}}$	388.00 ± 8.00	K	NIST Webbook
$T_{\text{fus}}$	396.00 ± 6.00	K	NIST Webbook
$T_{\text{fus}}$	394.00 ± 6.00	K	NIST Webbook
$T_{\text{fus}}$	392.00 ± 6.00	K	NIST Webbook
$T_{\text{fus}}$	373.00 ± 6.00	K	NIST Webbook
$T_{\text{fus}}$	391.00 ± 6.00	K	NIST Webbook

Property	Value	Unit	Source
$T_{\text{fus}}$	$373.00 \pm 6.00$	K	NIST Webbook
$T_{\text{fus}}$	$381.00 \pm 10.00$	K	NIST Webbook
$T_{\text{fus}}$	$383.00 \pm 10.00$	K	NIST Webbook
$T_{\text{fus}}$	$416.00 \pm 3.00$	K	NIST Webbook
$T_{\text{fus}}$	$400.00 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$395.00 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$391.00 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$408.00 \pm 5.00$	K	NIST Webbook
$T_{\text{fus}}$	$416.00 \pm 3.00$	K	NIST Webbook
$T_{\text{fus}}$	$406.00 \pm 10.00$	K	NIST Webbook
$T_{\text{fus}}$	$404.90 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$404.50 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$407.10 \pm 2.50$	K	NIST Webbook
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$T_{\text{fus}}$	$405.30 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$409.00 \pm 2.50$	K	NIST Webbook
$T_{\text{fus}}$	$407.30 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$405.25 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$403.50 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$406.80 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$405.90 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$409.30 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$407.10 \pm 2.00$	K	NIST Webbook

Property	Value	Unit	Source
$T_{\text{fus}}$	$404.70 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$404.80 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$406.50 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$407.90 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$407.50 \pm 2.50$	K	NIST Webbook
$T_{\text{fus}}$	$407.50 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$404.10 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$404.30 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$407.20 \pm 2.50$	K	NIST Webbook
$T_{\text{fus}}$	$406.70 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$406.30 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$407.60 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$407.20 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$402.20 \pm 4.00$	K	NIST Webbook
$T_{\text{fus}}$	$406.70 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$406.20 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$407.20 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$407.20 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$407.70 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$408.00 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$406.20 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$409.00 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$408.20 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$406.80 \pm 0.50$	K	NIST Webbook
$T_{\text{fus}}$	$406.80 \pm 0.50$	K	NIST Webbook
$T_{\text{fus}}$	$406.60 \pm 0.50$	K	NIST Webbook
$T_{\text{fus}}$	$407.80 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$402.10 \pm 4.00$	K	NIST Webbook

Property	Value	Unit	Source
$T_{\text{fus}}$	402.50 ± 4.00	K	NIST Webbook
$T_{\text{fus}}$	405.90 ± 3.00	K	NIST Webbook
$T_{\text{fus}}$	406.90 ± 3.00	K	NIST Webbook
$T_{\text{fus}}$	407.00 ± 3.00	K	NIST Webbook
$T_{\text{fus}}$	408.00 ± 1.50	K	NIST Webbook
$T_{\text{fus}}$	407.40 ± 0.50	K	NIST Webbook
$T_{\text{fus}}$	407.70 ± 0.50	K	NIST Webbook
$T_{\text{fus}}$	134.80 ± 0.50	K	NIST Webbook
$T_{\text{fus}}$	407.00 ± 3.00	K	NIST Webbook
$T_{\text{fus}}$	412.00 ± 4.00	K	NIST Webbook
$T_{\text{fus}}$	407.20 ± 2.00	K	NIST Webbook
$T_{\text{fus}}$	407.20 ± 2.00	K	NIST Webbook
$T_{\text{fus}}$	407.10 ± 3.00	K	NIST Webbook
$T_{\text{fus}}$	407.50 ± 2.00	K	NIST Webbook
$T_{\text{fus}}$	405.40 ± 1.00	K	NIST Webbook
$T_{\text{fus}}$	407.90 ± 2.00	K	NIST Webbook
$T_{\text{fus}}$	405.40 ± 1.00	K	NIST Webbook
$T_{\text{fus}}$	407.90 ± 2.00	K	NIST Webbook
$T_{\text{fus}}$	405.40 ± 1.00	K	NIST Webbook
$T_{\text{fus}}$	407.90 ± 2.00	K	NIST Webbook
$T_{\text{fus}}$	405.20 ± 2.00	K	NIST Webbook
$T_{\text{fus}}$	273.15 ± 5.00	K	NIST Webbook
$T_{\text{fus}}$	405.00 ± 3.00	K	NIST Webbook
$T_{\text{fus}}$	398.00 ± 6.00	K	NIST Webbook
$T_{\text{fus}}$	397.70 ± 3.00	K	NIST Webbook
$T_{\text{fus}}$	510.00 ± 4.00	K	NIST Webbook
$V_{\text{c}}$	0.48	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	313.39	J/molxK	659.32	Joback Method
$\eta$	0.00	Paxs	659.32	Joback Method
$\Delta_{fus} H$	29.17	kJ/mol	409.2	NIST Webbook
$\Delta_{fus} H$	31.01	kJ/mol	412.7	NIST Webbook
$\Delta_{fus} H$	29.80	kJ/mol	414.0	NIST Webbook

## 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/C9H8O4/c1-6\(10\)13-8-5-3-2-4-7\(8\)9\(11\)12/h2-5H,1H3,\(H,11,12\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12))

**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).

$\Delta_{fus} H$ : Enthalpy of fusion at a given temperature (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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