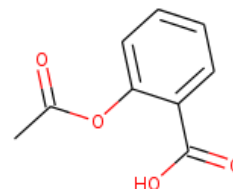


Benzoic acid, 2-(acetyloxy)-

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_{boil} | 659.32 | K | Joback Method |
| T_c | 868.49 | K | Joback Method |

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

| Property | Value | Unit | Source |
|------------------|--------------------|------|--------------|
| T_{fus} | 373.00 ± 6.00 | K | NIST Webbook |
| T_{fus} | 381.00 ± 10.00 | K | NIST Webbook |
| T_{fus} | 383.00 ± 10.00 | K | NIST Webbook |
| T_{fus} | 416.00 ± 3.00 | K | NIST Webbook |
| T_{fus} | 400.00 ± 2.00 | K | NIST Webbook |
| T_{fus} | 395.00 ± 2.00 | K | NIST Webbook |
| T_{fus} | 391.00 ± 2.00 | K | NIST Webbook |
| T_{fus} | 408.00 ± 5.00 | K | NIST Webbook |
| T_{fus} | 416.00 ± 3.00 | K | NIST Webbook |
| T_{fus} | 406.00 ± 10.00 | K | NIST Webbook |
| T_{fus} | 404.90 ± 2.00 | K | NIST Webbook |
| T_{fus} | 404.50 ± 2.00 | K | NIST Webbook |
| T_{fus} | 407.10 ± 2.50 | K | NIST Webbook |
| T_{fus} | 406.40 ± 2.00 | K | NIST Webbook |
| T_{fus} | 407.80 ± 2.00 | K | NIST Webbook |
| T_{fus} | 407.00 ± 2.50 | K | NIST Webbook |
| T_{fus} | 404.50 ± 2.00 | K | NIST Webbook |
| T_{fus} | 404.30 ± 2.00 | K | NIST Webbook |
| T_{fus} | 405.80 ± 2.00 | K | NIST Webbook |
| T_{fus} | 405.30 ± 2.00 | K | NIST Webbook |
| T_{fus} | 409.00 ± 2.50 | K | NIST Webbook |
| T_{fus} | 407.30 ± 2.00 | K | NIST Webbook |
| T_{fus} | 405.25 ± 2.00 | K | NIST Webbook |
| T_{fus} | 403.50 ± 2.00 | K | NIST Webbook |
| T_{fus} | 406.80 ± 2.00 | K | NIST Webbook |
| T_{fus} | 405.90 ± 2.00 | K | NIST Webbook |
| T_{fus} | 409.30 ± 2.00 | K | NIST Webbook |
| T_{fus} | 407.10 ± 2.00 | K | NIST Webbook |

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

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

Temperature Dependent Properties

| Property | Value | Unit | Temperature (K) | Source |
|------------------|--------|---------|-----------------|---------------|
| $C_{p,gas}$ | 313.39 | J/molxK | 659.32 | Joback Method |
| η | 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

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).

η : 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 (m³/kg-mol).

Latest version available from:

<https://www.cheméo.com/cid/43-227-2/Benzoic%20acid%2C%202-%28acetyloxy%29->

Generated by Cheméo on Fri, 20 Apr 2018 04:44:45 +0000.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.