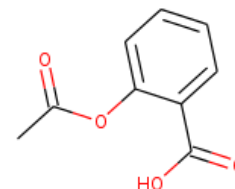


Benzoic acid, 2-(acetyloxy)-

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
$\log P_{\text{oct/wat}}$	1.310		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}	0.480	$\text{m}^3/\text{kg}\cdot\text{mol}$	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	313.39	J/molxK	659.32	Joback Method
η	0.0000687	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).

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