

Benzoic acid, 4-(acetyloxy)-

Other names:	4-(acetyloxy)benzoic acid 4-Acetate-benzoic acid 4-Carboxyphenyl acetate 4-acetoxybenzoic acid Benzoic acid, p-hydroxy-, acetate NSC 11340 O-Acetyl-p-hydroxybenzoic acid p-Acetoxybenzoic acid p-Acetyloxybenzoic acid p-Carboxyphenyl acetate p-Hydroxybenzoic acid acetate
Inchi:	InChI=1S/C9H8O4/c1-6(10)13-8-4-2-7(3-5-8)9(11)12/h2-5H,1H3,(H,11,12)
InchiKey:	GDBUZIKSJGRBJP-UHFFFAOYSA-N
Formula:	C9H8O4
SMILES:	CC(=O)Oc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	180.16
CAS:	2345-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-371.98	kJ/mol	Joback Method
hf	-513.64	kJ/mol	Joback Method
hfus	21.19	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Joback Method
ie	9.10 ± 0.20	eV	NIST Webbook
log10ws	-1.85		Crippen Method
logp	1.310		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	659.32	K	Joback Method
tc	868.49	K	Joback Method
tf	413.04	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.72	J/mol×K	833.63	Joback Method
cpg	358.88	J/mol×K	868.49	Joback Method
cpg	313.39	J/mol×K	659.32	Joback Method
cpg	322.42	J/mol×K	694.18	Joback Method
cpg	330.85	J/mol×K	729.04	Joback Method
cpg	338.71	J/mol×K	763.90	Joback Method
cpg	346.00	J/mol×K	798.77	Joback Method
dvisc	0.0000688	Pa×s	659.32	Joback Method
dvisc	0.0000976	Pa×s	618.27	Joback Method
dvisc	0.0015914	Pa×s	413.04	Joback Method
dvisc	0.0007440	Pa×s	454.09	Joback Method
dvisc	0.0003946	Pa×s	495.13	Joback Method
dvisc	0.0002306	Pa×s	536.18	Joback Method
dvisc	0.0001455	Pa×s	577.23	Joback Method
hfust	26.35	kJ/mol	467.20	NIST Webbook
hfust	26.35	kJ/mol	467.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2345348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 3,5-Dimethoxybenzoic Acid, 4-Cyanobenzoic Acid, 4-Acetoxybenzoic Acid, 3,5-Diaminobenzoic Acid, and 2,4-Dichlorobenzoic Acid in Ethanol:	https://www.doi.org/10.1021/je900190n https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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