4-hydroxybenzoic acid

Other names:	4-carboxyphenol
	Benzoic acid, 4-hydroxy-
	p-hydroxybenzoic acid
	p-salicylic acid
Inchi:	InChI=1S/C7H6O3/c8-6-3-1-5(2-4-6)7(9)10/h1-4,8H,(H,9,10)
InchiKey:	FJKROLUGYXJWQN-UHFFFAOYSA-N
Formula:	C7H6O3
SMILES:	O=C(O)c1ccc(O)cc1
Mol. weight [g/mol]:	138.12
CAS:	99-96-7

Physical Properties

Property code	Value	Unit	Source
chs	-3017.60 ± 0.50	kJ/mol	NIST Webbook
chs	-3005.40 ± 2.10	kJ/mol	NIST Webbook
gf	-299.89	kJ/mol	Joback Method
hf	-480.50	kJ/mol	NIST Webbook
hf	-492.60 ± 2.20	kJ/mol	NIST Webbook
hfs	-606.60 ± 2.10	kJ/mol	NIST Webbook
hfs	-594.50 ± 1.00	kJ/mol	NIST Webbook
hfus	19.40	kJ/mol	Joback Method
hsub	114.00	kJ/mol	NIST Webbook
hsub	114.05 ± 0.69	kJ/mol	NIST Webbook
hsub	117.00 ± 0.50	kJ/mol	NIST Webbook
hsub	116.10 ± 0.40	kJ/mol	NIST Webbook
hsub	114.10 ± 0.70	kJ/mol	NIST Webbook
hvap	69.89	kJ/mol	Joback Method
ie	9.20 ± 0.20	eV	NIST Webbook
log10ws	-1.42		Aqueous Solubility Prediction Method
logp	1.090		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	6349.11	kPa	Joback Method
rinpol	1558.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1577.00		NIST Webbook

rinpol	1558.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1537.70		NIST Webbook
ss	175.70	J/mol×K	NIST Webbook
tb	612.91	K	Joback Method
tc	833.23	K	Joback Method
tf	488.40	K	Aqueous Solubility Prediction Method
tf	488.10 ± 0.50	K	NIST Webbook
tf	489.00 ± 1.00	K	NIST Webbook
tf	489.35 ± 0.70	K	NIST Webbook
tf	486.00 ± 4.00	K	NIST Webbook
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.10	J/mol×K	612.91	Joback Method
cpg	269.96	J/mol×K	833.23	Joback Method
cpg	264.74	J/mol×K	796.51	Joback Method
cpg	259.25	J/mol×K	759.79	Joback Method
cpg	253.40	J/mol×K	723.07	Joback Method
cpg	247.14	J/mol×K	686.35	Joback Method
cpg	240.40	J/mol×K	649.63	Joback Method
cps	191.00	J/mol×K	395.80	Determination of the activity of a molecular solute in saturated solution
cps	204.50	J/mol×K	430.80	Determination of the activity of a molecular solute in saturated solution
cps	202.20	J/mol×K	425.80	Determination of the activity of a molecular solute in saturated solution
cps	200.40	J/mol×K	420.80	Determination of the activity of a molecular solute in saturated solution

cps	198.70	J/mol×K	415.80	Determination of the activity of a molecular solute in saturated solution
cps	197.00	J/mol×K	410.80	Determination of the activity of a molecular solute in saturated solution
cps	195.10	J/mol×K	405.80	Determination of the activity of a molecular solute in saturated solution
cps	193.10	J/mol×K	400.80	Determination of the activity of a molecular solute in saturated solution
cps	207.10	J/mol×K	435.80	Determination of the activity of a molecular solute in saturated solution
cps	209.50	J/mol×K	440.80	Determination of the activity of a molecular solute in saturated solution
cps	211.60	J/mol×K	445.80	Determination of the activity of a molecular solute in saturated solution
cps	213.80	J/mol×K	450.80	Determination of the activity of a molecular solute in saturated solution
cps	215.90	J/mol×K	455.80	Determination of the activity of a molecular solute in saturated solution
cps	218.20	J/mol×K	460.70	Determination of the activity of a molecular solute in saturated solution
cps	138.90	J/mol×K	280.80	Determination of the activity of a molecular solute in saturated solution
cps	141.30	J/mol×K	285.80	Determination of the activity of a molecular solute in saturated solution

cps	143.50	J/mol×K	290.80	Determination of the activity of a molecular solute in saturated solution
cps	145.70	J/mol×K	295.80	Determination of the activity of a molecular solute in saturated solution
cps	148.00	J/mol×K	300.70	Determination of the activity of a molecular solute in saturated solution
cps	149.70	J/mol×K	305.80	Determination of the activity of a molecular solute in saturated solution
cps	151.80	J/mol×K	310.80	Determination of the activity of a molecular solute in saturated solution
cps	154.60	J/mol×K	315.80	Determination of the activity of a molecular solute in saturated solution
cps	156.40	J/mol×K	320.80	Determination of the activity of a molecular solute in saturated solution
cps	158.70	J/mol×K	325.80	Determination of the activity of a molecular solute in saturated solution
cps	161.40	J/mol×K	330.80	Determination of the activity of a molecular solute in saturated solution
cps	163.80	J/mol×K	335.80	Determination of the activity of a molecular solute in saturated solution
cps	166.30	J/mol×K	340.80	Determination of the activity of a molecular solute in saturated solution
cps	168.60	J/mol×K	345.80	Determination of the activity of a molecular solute in saturated solution

cps	171.10	J/mol×K	350.80	Determination of the activity of a molecular solute in saturated solution
cps	173.40	J/mol×K	355.80	Determination of the activity of a molecular solute in saturated solution
cps	175.50	J/mol×K	360.80	Determination of the activity of a molecular solute in saturated solution
cps	177.80	J/mol×K	365.70	Determination of the activity of a molecular solute in saturated solution
cps	180.00	J/mol×K	370.70	Determination of the activity of a molecular solute in saturated solution
cps	182.00	J/mol×K	375.70	Determination of the activity of a molecular solute in saturated solution
cps	184.40	J/mol×K	380.80	Determination of the activity of a molecular solute in saturated solution
cps	186.70	J/mol×K	385.80	Determination of the activity of a molecular solute in saturated solution
cps	188.90	J/mol×K	390.80	Determination of the activity of a molecular solute in saturated solution
cps	155.20	J/mol×K	283.80	NIST Webbook
dvisc	0.0000161	Pa×s	612.91	Joback Method
dvisc	0.0004096	Pa×s	450.10	Joback Method
dvisc	0.0001801	Pa×s	482.66	Joback Method
dvisc	0.0000879	Pa×s	515.23	Joback Method
dvisc	0.0000467	Pa×s	547.79	Joback Method
dvisc	0.0000266	Pa×s	580.35	Joback Method
dvisc	0.0010587	Pa×s	417.54	Joback Method
hfust	30.85	kJ/mol	489.00	NIST Webbook
hfust	31.40	kJ/mol	487.20	NIST Webbook
hfust	32.00	kJ/mol	488.00	NIST Webbook

hfust	30.90	kJ/mol	488.10	NIST Webbook
hfust	30.90	kJ/mol	488.10	NIST Webbook
hsubt	112.40 ± 0.70	kJ/mol	363.00	NIST Webbook
hsubt	116.30	kJ/mol	415.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The effect of temperature on the solubility of benzoic acid derivatives in water:	https://www.doi.org/10.1016/j.fluid.2006.10.014
Determination of the activity of a molecular solute in saturated solution: Solubilities of Benzoic Acid, p-Methylbenzoic Acid, m-Methylbenzoic Acid, o-Methylbenzoic Acid, p-Hydroxybenzoic Acid, and o-Nitrobenzoic Acid in 1-Octanol:	https://www.doi.org/10.1016/j.jct.2008.06.016
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume