3-hydroxybenzoic acid

Other names:	3-carboxyphenol
	benzoic acid, 3-hydroxy-
	m-hydroxybenzoic acid
	m-salicylic acid
Inchi:	InChI=1S/C7H6O3/c8-6-3-1-2-5(4-6)7(9)10/h1-4,8H,(H,9,10)
InchiKey:	IJFXRHURBJZNAO-UHFFFAOYSA-N
Formula:	C7H6O3
SMILES:	O=C(O)c1cccc(O)c1
Mol. weight [g/mol]:	138.12
CAS:	99-06-9

Physical Properties

Property code	Value	Unit	Source
chs	-3021.60 ± 0.40	kJ/mol	NIST Webbook
chs	-3017.90 ± 1.10	kJ/mol	NIST Webbook
gf	-299.89	kJ/mol	Joback Method
hf	-469.10 ± 1.30	kJ/mol	NIST Webbook
hf	-465.50	kJ/mol	NIST Webbook
hfs	-594.10 ± 1.10	kJ/mol	NIST Webbook
hfs	-590.50 ± 1.00	kJ/mol	NIST Webbook
hfus	19.40	kJ/mol	Joback Method
hsub	125.00 ± 0.74	kJ/mol	NIST Webbook
hsub	124.99 ± 0.74	kJ/mol	NIST Webbook
hsub	125.00	kJ/mol	NIST Webbook
hsub	118.30 ± 1.10	kJ/mol	NIST Webbook
hvap	69.89	kJ/mol	Joback Method
ie	9.20 ± 0.20	eV	NIST Webbook
log10ws	-1.08		Crippen Method
logp	1.090		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	6349.11	kPa	Joback Method
rinpol	1417.00		NIST Webbook
ss	177.00	J/mol×K	NIST Webbook
tb	612.91	K	Joback Method
tc	833.23	K	Joback Method
tf	472.00 ± 6.00	K	NIST Webbook
tf	364.00 ± 3.00	K	NIST Webbook

tf	472.00 ± 1.50	K	NIST Webbook
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.25	J/mol×K	759.79	Joback Method
cpg	269.96	J/mol×K	833.23	Joback Method
cpg	264.74	J/mol×K	796.51	Joback Method
cpg	233.10	J/mol×K	612.91	Joback Method
cpg	240.40	J/mol×K	649.63	Joback Method
cpg	247.14	J/mol×K	686.35	Joback Method
cpg	253.40	J/mol×K	723.07	Joback Method
cps	138.90	J/mol×K	290.50	Determination of the activity of a molecular solute in saturated solution
cps	157.30	J/mol×K	288.40	NIST Webbook
cps	207.50	J/mol×K	440.50	Determination of the activity of a molecular solute in saturated solution
cps	134.60	J/mol×K	280.40	Determination of the activity of a molecular solute in saturated solution
cps	136.80	J/mol×K	285.50	Determination of the activity of a molecular solute in saturated solution
cps	218.80	J/mol×K	460.40	Determination of the activity of a molecular solute in saturated solution
cps	141.20	J/mol×K	295.40	Determination of the activity of a molecular solute in saturated solution
cps	143.50	J/mol×K	300.40	Determination of the activity of a molecular solute in saturated solution

cps	145.80	J/mol×K	305.40	Determination of the activity of a molecular solute in saturated solution
cps	147.90	J/mol×K	310.40	Determination of the activity of a molecular solute in saturated solution
cps	150.20	J/mol×K	315.40	Determination of the activity of a molecular solute in saturated solution
cps	152.70	J/mol×K	320.40	Determination of the activity of a molecular solute in saturated solution
cps	155.00	J/mol×K	325.50	Determination of the activity of a molecular solute in saturated solution
cps	157.40	J/mol×K	330.50	Determination of the activity of a molecular solute in saturated solution
cps	159.70	J/mol×K	335.50	Determination of the activity of a molecular solute in saturated solution
cps	162.20	J/mol×K	340.50	Determination of the activity of a molecular solute in saturated solution
cps	164.50	J/mol×K	345.50	Determination of the activity of a molecular solute in saturated solution
cps	166.90	J/mol×K	350.40	Determination of the activity of a molecular solute in saturated solution
cps	169.10	J/mol×K	355.40	Determination of the activity of a molecular solute in saturated solution
cps	171.30	J/mol×K	360.40	Determination of the activity of a molecular solute in saturated solution

cps	209.90	J/mol×K	445.50	Determination of the activity of a molecular solute in saturated solution
cps	175.90	J/mol×K	370.40	Determination of the activity of a molecular solute in saturated solution
cps	177.90	J/mol×K	375.40	Determination of the activity of a molecular solute in saturated solution
cps	180.80	J/mol×K	380.40	Determination of the activity of a molecular solute in saturated solution
cps	183.80	J/mol×K	385.40	Determination of the activity of a molecular solute in saturated solution
cps	186.30	J/mol×K	390.50	Determination of the activity of a molecular solute in saturated solution
cps	188.70	J/mol×K	395.50	Determination of the activity of a molecular solute in saturated solution
cps	190.60	J/mol×K	400.50	Determination of the activity of a molecular solute in saturated solution
cps	192.60	J/mol×K	405.50	Determination of the activity of a molecular solute in saturated solution
cps	194.60	J/mol×K	410.50	Determination of the activity of a molecular solute in saturated solution
cps	196.60	J/mol×K	415.50	Determination of the activity of a molecular solute in saturated solution
cps	198.30	J/mol×K	420.50	Determination of the activity of a molecular solute in saturated solution

cps	200.30	J/mol×K	425.50	Determination of the activity of a molecular solute in saturated solution
cps	202.50	J/mol×K	430.50	Determination of the activity of a molecular solute in saturated solution
cps	205.00	J/mol×K	435.50	Determination of the activity of a molecular solute in saturated solution
cps	214.80	J/mol×K	455.50	Determination of the activity of a molecular solute in saturated solution
cps	173.70	J/mol×K	365.40	Determination of the activity of a molecular solute in saturated solution
cps	212.10	J/mol×K	450.50	Determination of the activity of a molecular solute in saturated solution
dvisc	0.0000161	Pa×s	612.91	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
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
hfust	36.50	kJ/mol	476.40	NIST Webbook
hfust	26.20	kJ/mol	475.10	NIST Webbook
hsubt	123.50 ± 0.74	kJ/mol	363.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Determination of the activity of a molecular solute in saturated solution: https://www.doi.org/10.1016/j.jct.2008.06.016

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99069&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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