Salicylic acid

Other names:

2-Carboxyphenol
2-Hydroxybenzenecarboxylic acid
2-Hydroxybenzoic acid
7681-06-3
8052-31-1
Acido salicilico
Advanced pain relief callus removers
Advanced pain relief corn removers
Benzoic acid, 2-hydroxy-
Benzoic acid, o-hydroxy-
Clear away wart remover
Compound W
Domerine
Dr. Scholl's Callus Removers
Dr. Scholl's Corn Removers
Dr. Scholl's Wart Remover Kit
Duofil Wart Remover
Duofilm
Duoplant
Fostex
Freezone
Ionil
Ionil plus
Keralyt
Kyselina 2-hydroxybenzoova
Kyselina salicylova
NSC 180
Orthohydroxybenzoic acid
Pernox
Phenol-2-carboxylic acid
Psoriacid-S-Stift
Retarder SAX
Retarder W
Rutranex
Salicyclic acid
Salicylic acid & Sulfur Soap
Salicylic acid collodion
Salicylic acid soap
Saligel
Salonil

	Sebucare
	Sebulex
	Stri-Dex
	Trans-Ver-Sal
	component of Fostex medicated bar and cream
	component of Keralyt
	component of Solarcaine first aid spray
	component of Tinver
	o-Carboxyphenol
	o-Hydroxybenzoic acid
Inchi:	InChI=1S/C7H6O3/c8-6-4-2-1-3-5(6)7(9)10/h1-4,8H,(H,9,10)
InchiKey:	YGSDEFSMJLZEOE-UHFFFAOYSA-N
Formula:	C7H6O3
SMILES:	O=C(O)c1ccccc1O
Mol. weight [g/mol]:	138.12
CAS:	69-72-7

Physical Properties

Property code	Value	Unit	Source
chs	-3024.70	kJ/mol	NIST Webbook
chs	-3029.00 ± 0.40	kJ/mol	NIST Webbook
chs	-3026.80	kJ/mol	NIST Webbook
chs	-3026.80	kJ/mol	NIST Webbook
chs	-3023.60	kJ/mol	NIST Webbook
chs	-3024.70	kJ/mol	NIST Webbook
chs	-3022.90	kJ/mol	NIST Webbook
chs	-3029.60	kJ/mol	NIST Webbook
chs	-3025.00	kJ/mol	NIST Webbook
chs	-3027.29	kJ/mol	NIST Webbook
chs	-3022.40 ± 0.50	kJ/mol	NIST Webbook
chs	-3020.00 ± 1.30	kJ/mol	NIST Webbook
gf	-299.89	kJ/mol	Joback Method
hf	-489.00	kJ/mol	NIST Webbook
hf	-495.80 ± 1.40	kJ/mol	NIST Webbook
hf	-493.40	kJ/mol	NIST Webbook
hfs	-592.10 ± 1.30	kJ/mol	NIST Webbook
hfs	-589.70 ± 1.10	kJ/mol	NIST Webbook
hfs	-585.30	kJ/mol	NIST Webbook
hfus	27.09	kJ/mol	Solubility and Melting Properties of Salicylic Acid

hfus	24.06	kJ/mol	Solubility of salicylic acid in pure alcohols at different temperatures
hsub	96.30	kJ/mol	NIST Webbook
hsub	96.27 ± 0.49	kJ/mol	NIST Webbook
hsub	95.10 ± 0.40	kJ/mol	NIST Webbook
hsub	95.70 ± 0.10	kJ/mol	NIST Webbook
hsub	94.40 ± 0.40	kJ/mol	NIST Webbook
hsub	81.75	kJ/mol	NIST Webbook
hsub	96.30 ± 0.50	kJ/mol	NIST Webbook
hvap	69.89	kJ/mol	Joback Method
log10ws	-1.85		Aqueous Solubility Prediction Method
log10ws	-1.93		Aqueous Solubility Prediction Method
logp	1.090		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	6349.11	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1295.80		NIST Webbook
rinpol	1295.80		NIST Webbook
ss	172.40	J/mol×K	NIST Webbook
ss	178.20	J/mol×K	NIST Webbook
tb	612.91	K	Joback Method
tc	833.23	K	Joback Method

tf	432.70	K	Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements
tf	430.00 ± 4.00	K	NIST Webbook
tf	431.45 ± 0.50	K	NIST Webbook
tf	432.00 ± 1.50	K	NIST Webbook
tf	432.10 ± 0.80	K	NIST Webbook
tf	432.15	K	Liquid pharmaceuticals formulation by eutectic formation
tf	431.92	K	Aqueous Solubility Prediction Method
tf	431.92	K	Aqueous Solubility Prediction Method
tf	432.00 ± 0.80	K	NIST Webbook
tf	432.10 ± 0.80	K	NIST Webbook
tf	432.20 ± 0.80	K	NIST Webbook
tf	432.00	K	Polar Mixed-Solid Solute Systems in Supercritical Carbon Dioxide: Entrainer Effect and Its Influence on Solubility and Selectivity
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	156.20	J/mol×K	350.40	Determination of the activity of a molecular solute in saturated solution
cps	172.10	J/mol×K	390.40	Determination of the activity of a molecular solute in saturated solution

cps	168.00	J/mol×K	380.40	Determination of the activity of a molecular solute in saturated solution
cps	165.90	J/mol×K	375.40	Determination of the activity of a molecular solute in saturated solution
cps	164.20	J/mol×K	370.40	Determination of the activity of a molecular solute in saturated solution
cps	162.30	J/mol×K	365.40	Determination of the activity of a molecular solute in saturated solution
cps	160.30	J/mol×K	360.40	Determination of the activity of a molecular solute in saturated solution
cps	158.20	J/mol×K	355.40	Determination of the activity of a molecular solute in saturated solution
cps	173.80	J/mol×K	395.50	Determination of the activity of a molecular solute in saturated solution
cps	175.60	J/mol×K	400.50	Determination of the activity of a molecular solute in saturated solution
cps	177.50	J/mol×K	405.50	Determination of the activity of a molecular solute in saturated solution
cps	160.90	J/mol×K	298.15	NIST Webbook
cps	104.20	J/mol×K	293.00	NIST Webbook
cps	159.40	J/mol×K	288.60	NIST Webbook
cps	128.50	J/mol×K	280.40	Determination of the activity of a molecular solute in saturated solution
cps	130.00	J/mol×K	285.50	Determination of the activity of a molecular solute in saturated solution

cps	131.60	J/mol×K	290.50	Determination of the activity of a molecular solute in saturated solution
cps	133.50	J/mol×K	295.40	Determination of the activity of a molecular solute in saturated solution
cps	135.40	J/mol×K	300.40	Determination of the activity of a molecular solute in saturated solution
cps	137.40	J/mol×K	305.40	Determination of the activity of a molecular solute in saturated solution
cps	139.40	J/mol×K	310.40	Determination of the activity of a molecular solute in saturated solution
cps	141.40	J/mol×K	315.40	Determination of the activity of a molecular solute in saturated solution
cps	143.50	J/mol×K	320.40	Determination of the activity of a molecular solute in saturated solution
cps	145.50	J/mol×K	325.40	Determination of the activity of a molecular solute in saturated solution
cps	147.60	J/mol×K	330.40	Determination of the activity of a molecular solute in saturated solution
cps	149.80	J/mol×K	335.40	Determination of the activity of a molecular solute in saturated solution
cps	151.80	J/mol×K	340.40	Determination of the activity of a molecular solute in saturated solution
cps	154.10	J/mol×K	345.40	Determination of the activity of a molecular solute in saturated solution

cps	170.10	J/mol×K	385.40	Determination of the activity of a molecular solute in saturated solution
dvisc	0.0000161	Pa×s	612.91	Joback Method
dvisc	0.0000266	Pa×s	580.35	Joback Method
dvisc	0.0000467	Pa×s	547.79	Joback Method
dvisc	0.0000879	Pa×s	515.23	Joback Method
dvisc	0.0001801	Pa×s	482.66	Joback Method
dvisc	0.0004096	Pa×s	450.10	Joback Method
dvisc	0.0010587	Pa×s	417.54	Joback Method
hfust	24.45	kJ/mol	431.10	NIST Webbook
hfust	27.10	kJ/mol	434.10	NIST Webbook
hfust	23.05	kJ/mol	432.50	NIST Webbook
hfust	24.60	kJ/mol	431.80	NIST Webbook
hfust	24.60	kJ/mol	431.80	NIST Webbook
hsubt	95.10 ± 0.50	kJ/mol	333.00	NIST Webbook
hsubt	95.70 ± 0.80	kJ/mol	315.50	NIST Webbook
hsubt	93.20 ± 0.80	kJ/mol	322.00	NIST Webbook
hsubt	99.00 ± 2.00	kJ/mol	313.00	NIST Webbook
hsubt	94.80 ± 0.40	kJ/mol	388.00	NIST Webbook
hsubt	95.10 ± 0.40	kJ/mol	388.00	NIST Webbook
hsubt	94.90 ± 0.40	kJ/mol	322.00	NIST Webbook
hvapt	79.40	kJ/mol	474.50	NIST Webbook
sfust	56.90	J/mol×K	431.80	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	484.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.74158e+02
Coeff. B	-3.34417e+04

Coeff. C	-6.61599e+01
Coeff. D	3.08189e-05
Temperature range (K), min.	431.75
Temperature range (K), max.	739.00

Sources

Synthesis, Characterization and Standard Molar Enthalpy of Formation of Sm(C7H5O3)2·(C9H6NO):	https://www.doi.org/10.1016/j.tca.2007.10.003
Solubility of Benzoic and Salicylic Acids in Subcritical Water at Temperatures Ranging from (298 to 473) K:	https://www.doi.org/10.1021/je900769d
Solubility of Glycyrrhizin in supercritical carbon dioxide with and without cosolvent:	https://www.doi.org/10.1021/je5011328
Solubility of Salicylic Acid in Water, Ethanol, Carbon Tetrachloride, Ethyl Acetate, and Xylene:	https://www.doi.org/10.1021/je7004962
Solubility of Benzoin in Six Monosolvents and in Some Binary Solvent Mixtures at Various Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00238
Polar Mixed-Solid Solute Systems in Supercritical Carbon Dioxide: Entrainer Effect and Its Influence on Solubility and Selectivity:	https://www.doi.org/10.1021/je700486g
Solubility of salicylic acid in pure alcohols at different temperatures:	https://www.doi.org/10.1016/j.jct.2012.09.006
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=982
Determination and Correlation of Solubility and Thermodynamic Properties of trans-Cinnamyl Alcohol in Pure and Binary Solvents from 253.15 K to 293.15 K:	https://www.doi.org/10.1021/acs.jced.7b00665
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
Determination of the activity of a molecular solute in saturated solution:	https://www.doi.org/10.1016/j.jct.2008.06.016
Thermochemical Analysis on Rare Earth Complex of Gadolinium with Salicylic acid and 8-hydroxyquinoline:	https://www.doi.org/10.1016/j.tca.2012.08.027
Solubility of 2-Hydroxybenzoic Acid in Water, 1-Propanol, 2-Propanol, and 2-Propanone at (298.2 to 338.2) K and Their Aqueous Binary Mixtures at 298.2 K:	https://www.doi.org/10.1021/je300980k
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69727&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubilities of Salicylic Acid in Pure Solvents and Binary Mixtures Containing Cosolvent:	https://www.doi.org/10.1021/je800475d
Synthesis, characterization and standard molar enthalpy of formation of La(C7H5O3)2·(C9H6NO):	https://www.doi.org/10.1016/j.tca.2005.10.015
Construction, calibration and testing of a micro-combustion calorimeter:	https://www.doi.org/10.1016/j.jct.2006.03.001
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility and Melting Properties of Salicylic Acid:	https://www.doi.org/10.1021/je060134d
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solubility of 4-Methylsulfonylacetophenone in Nine Pure Solvents and (Ethyl Acetate + n-Hexane) Binary Solvent Mixtures from 278.15 K to 323.15 K:	https://www.doi.org/10.1021/acs.jced.6b00617
Strategy for extractant residual reduction: Experimental and computational investigation of fluorinated phosphate:	https://www.doi.org/10.1016/j.fluid.2017.06.026
Solubility of salicylic acid in water + salt (NaCl, KCl, NaBr, Na2SO4 and K2SO4) at 293.5 to 313.3 K:	https://www.doi.org/10.1016/j.fluid.2012.06.024
Liquid pharmaceuticals formulation by eutectic formation:	https://www.doi.org/10.1016/j.fluid.2017.05.009
Measurement and Correlation of the Solubility of 2,6-Dihydroxybenzoic Acid in Alcohols and Binary Solvents:	https://www.doi.org/10.1021/acs.jced.6b00957
Calibration and testing of an isoperibolic micro-combustion calorimeter developed to measure the enthalpy of combustion of organic compounds containing C, H, O and N:	https://www.doi.org/10.1016/j.jct.2012.12.020

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume