BENZALDEHYDE, 2-HYDROXY-

Other names:	2-Formylphenol
	2-Hydroxy benzaldehyde (salicylaldehyde)
	2-hydroxybenzaldehyde
	Benzaldehyde, o-hydroxy-
	NSC 49178
	SAH
	Salicylal
	Salicylaldehyde (2-hydroxybenzaldehyde)
	Salicylic aldehyde
	o-Formylphenol
	o-Hydroxybenzaldehyde
	salicylaldehyde
Inchi:	InChI=1S/C7H6O2/c8-5-6-3-1-2-4-7(6)9/h1-5,9H
InchiKey:	SMQUZDBALVYZAC-UHFFFAOYSA-N
Formula:	C7H6O2
SMILES:	O=Cc1ccccc1O
Mol. weight [g/mol]:	122.12
CAS:	90-02-8

Physical Properties

Property code	Value	Unit	Source
hf	-239.97	kJ/mol	Cheméo Relay (1.0)
hfus	16.00	kJ/mol	Joback Method
hvap	53.30 ± 0.30	kJ/mol	NIST Webbook
hvap	50.40 ± 1.30	kJ/mol	NIST Webbook
ie	8.63	eV	Cheméo Relay (1.0)
log10ws	-0.86		Aqueous Solubility Prediction Method
logp	1.205		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
rinpol	1057.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1047.60		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1062.00		NIST Webbook

rinpol	1074.00	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1008.00	NIST Webbook
rinpol	1003.00	NIST Webbook
rinpol	1031.00	NIST Webbook
rinpol	1027.00	NIST Webbook
rinpol	1057.00	NIST Webbook
rinpol	1013.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1041.00	NIST Webbook
rinpol	1041.00	NIST Webbook
rinpol	1041.00	NIST Webbook
rinpol	1011.00	NIST Webbook
rinpol	1026.00	NIST Webbook
rinpol	1031.00	NIST Webbook
rinpol	1021.00	NIST Webbook
rinpol	1025.00	NIST Webbook
rinpol	1024.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1063.00	NIST Webbook
rinpol	1062.00	NIST Webbook
rinpol	1041.30	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1041.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1011.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1008.00	NIST Webbook
rinpol	1005.00	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1055.00	NIST Webbook
rinpol	1008.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1041.40	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1054.00	NIST Webbook
rinpol	1013.00	NIST Webbook
rinpol	1072.00	NIST Webbook

ripol	1682.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1699.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1674.00		NIST Webbook
tb	470.20	K	NIST Webbook
tb	470.15 ± 1.00	K	NIST Webbook
tc	790.07	K	Cheméo Relay (1.0)
tf	272.30	K	Vapor Pressures and Gibbs Energies of Formation of the Three Hydroxybenzaldehydes
tf	269.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.05	J/mol×K	593.53	Joback Method
cpg	242.09	J/mol×K	749.54	Joback Method
cpg	236.10	J/mol×K	710.54	Joback Method
cpg	229.65	J/mol×K	671.53	Joback Method
cpg	222.66	J/mol×K	632.53	Joback Method
cpg	197.64	J/mol×K	515.52	Joback Method
cpg	206.73	J/mol×K	554.52	Joback Method
dvisc	0.0031017	Pa×s	348.79	Joback Method
dvisc	0.0014153	Pa×s	376.58	Joback Method
dvisc	0.0007194	Pa×s	404.37	Joback Method
dvisc	0.0003989	Pa×s	432.15	Joback Method
dvisc	0.0002375	Pa×s	459.94	Joback Method
dvisc	0.0001500	Pa×s	487.73	Joback Method
dvisc	0.0000996	Pa×s	515.52	Joback Method
hfust	13.30	kJ/mol	278.70	NIST Webbook
hvapt	49.60	kJ/mol	388.00	NIST Webbook
hvapt	30.60	kJ/mol	426.50	NIST Webbook
hvapt	63.30	kJ/mol	298.15	Thermochemical studies on salicylaldehyde and salicylamide
rhol	1162.50	kg/m3	298.15	Liquid-liquid equilibria for (2-hydroxy benzaldehyde + n-alkane) mixtures. Intermolecular and proximity effects in systems containing hydroxyl and aldehyde groups

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.71544e+01
Coeff. B	-5.86328e+03
Coeff. C	-2.48700e+00
Temperature range (K), min.	350.11
Temperature range (K), max.	497.57

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.31045e+01
Coeff. B	-8.28909e+03
Coeff. C	-8.49841e+00
Coeff. D	6.54847e-06
Temperature range (K), min.	266.15
Temperature range (K), max.	680.00

Sources

Thermochemical studies on salicylaldehyde and salicylamide:	https://www.doi.org/10.1016/j.jct.2007.03.006
Liquid-liquid equilibria for (2-hydroxy benzaldehyde + n-alkane) mixtures.	https://www.doi.org/10.1016/j.jct.2019.04.002
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Intermolecular and proximity effects in systems containing hydroxyl and aldehyde groups:	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Cheméo Relay (1.0):	
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1246
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Henry s Law Constants of Some Aromatic Aldehydes and Ketones Measured by an Internal Standard Method:	https://www.doi.org/10.1021/je700612b
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90028&Units=SI
Thermochemical study on the Schiff base[H2salen = N,N -bis(salicylidene) ethylenediamine] and its	https://www.doi.org/10.1016/j.tca.2013.07.004
Vapor Pressures and Gibbs Energies of Formation of the Three Hydroxybenzaldehydes:	https://www.doi.org/10.1021/acs.jced.7b00227
binuclear copper (II) complex:	
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1246
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point