

Vanillin

Other names:	2-Methoxy-4-formylphenol 3-Methoxy-4-hydroxybenzaldehyde 3-Methoxy-4-hydroxybenzaldehyde (vanillin) 4-Formyl-2-methoxyphenol 4-Hydroxy-3-methoxybenzaldehyde 4-Hydroxy-5-methoxybenzaldehyde 4-Hydroxy-m-anisaldehyde 4-hydroxy-3-methoxybenzaldehyde (vanillin) Benzaldehyde, 4-hydroxy-3-methoxy- Lioxin Methylprotcatechuic aldehyde Methylprotocatechuic aldehyde NSC 15351 Protocatechualdehyde, methyl- Vanilin Vanilla Vanillaldehyde Vanillic aldehyde Zimco m-Anisaldehyde, 4-hydroxy- m-Methoxy-p-hydroxybenzaldehyde p-Hydroxy-m-methoxybenzaldehyde p-Vanillin vanillin (3-methoxy-4-hydroxy- benzaldehyde)
Inchi:	InChI=1S/C8H8O3/c1-11-8-4-6(5-9)2-3-7(8)10/h2-5,10H,1H3
InchiKey:	MWOOGOJBHIARFG-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	COc1cc(C=O)ccc1O
Mol. weight [g/mol]:	152.15
CAS:	121-33-5

Physical Properties

Property code	Value	Unit	Source
chs	-3828.00	kJ/mol	NIST Webbook
gf	-239.88	kJ/mol	Joback Method
hf	-378.50	kJ/mol	Joback Method

hfus	23.96			Influence of the aromatic ring substituents on phase equilibria of vanillins in binary systems with CO2
hvac	66.90			
log10ws	-1.15			
logp	1.213			
mccol	113.130			
pc	4665.71			
rinpol	1372.86			
rinpol	1353.19			
rinpol	1357.77			
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rinpol	1367.56			
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tb	565.80	K	Joback Method
tc	793.56	K	Joback Method
tf	355.10 ± 0.80	K	NIST Webbook
tf	354.90	K	Aqueous Solubility Prediction Method
tf	355.95 ± 1.50	K	NIST Webbook
tf	355.40 ± 0.80	K	NIST Webbook
tf	354.90 ± 1.00	K	NIST Webbook
tf	354.30 ± 0.80	K	NIST Webbook
tf	355.10 ± 0.80	K	NIST Webbook
tf	355.10 ± 0.80	K	NIST Webbook
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.74	J/mol×K	565.80	Joback Method
cpg	269.43	J/mol×K	603.76	Joback Method
cpg	278.48	J/mol×K	641.72	Joback Method
cpg	286.94	J/mol×K	679.68	Joback Method
cpg	294.87	J/mol×K	717.64	Joback Method
cpg	302.31	J/mol×K	755.60	Joback Method
cpg	309.32	J/mol×K	793.56	Joback Method
dvisc	0.0005373	Pa×s	423.31	Joback Method
dvisc	0.0010401	Pa×s	394.81	Joback Method
dvisc	0.0003017	Pa×s	451.81	Joback Method
dvisc	0.0001814	Pa×s	480.30	Joback Method
dvisc	0.0001155	Pa×s	508.80	Joback Method
dvisc	0.0000771	Pa×s	537.30	Joback Method

dvisc	0.0000536	Pa×s	565.80	Joback Method
hfust	22.40	kJ/mol	355.40	NIST Webbook
hsubt	88.70	kJ/mol	323.00	NIST Webbook
hvapt	66.90	kJ/mol	469.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.69294e+02
Coeff. B	-1.67466e+04
Coeff. C	-2.17064e+01
Coeff. D	8.35934e-06
Temperature range (K), min.	355.00
Temperature range (K), max.	777.00

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C121335&Units=SI>

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Infinite Dilution Binary Diffusion Coefficients for Compounds Derived from Binary Systems in Water and 1-Methyl-2-pyrrolidone at 298.15 K and Systems Containing 298.15 and 309.2 K: Salicylic Acid, Gallic Acid, Carbon Syringic Acid, and Protocatechuic Acid in Aqueous Solutions from (293.15 to 318.15) K: Vapor-Liquid Equilibrium Behaviors of Vanillin in 1-Butanol, 2-Butanol, and 1-Methyl-1-propanol:

<https://www.doi.org/10.1021/je301060a>
<https://www.doi.org/10.1021/acs.jced.6b00322>
<https://www.doi.org/10.1021/je800205e>
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<https://www.doi.org/10.1021/je700063c>
<https://www.cheric.org/files/research/kdb/mol/mol1249.mol>

Temperature and salt addition effects on the solubility behaviour of some construction powder in water phase diagrams in ternary systems by the liquid-liquid phase separation and crystallization of vanillin in 1-propanol/water solution:

<https://www.doi.org/10.1016/j.jct.2006.06.014>
<https://www.doi.org/10.1016/j.tca.2006.02.017>
<https://www.doi.org/10.1016/j.fluid.2015.09.011>

Vapor-Liquid Equilibrium Behaviors of Coumarin and Vanillin in Ethanol, McGowan Method-Propanol:	https://www.doi.org/10.1021/je0505164 http://link.springer.com/article/10.1007/BF02311772
Phase equilibria of phenolic compounds in water or ethanol: Joback Method:	https://www.doi.org/10.1016/j.fluid.2017.09.008 https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Influence of the aromatic ring substituents on phase equilibria of vanillins in binary systems with CO ₂ :	https://www.doi.org/10.1016/j.fluid.2004.12.012

Legend

chs:	Standard solid enthalpy of combustion
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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