

Ethyl Vanillin

Other names: 2-Ethoxy-4-formylphenol
3-Ethoxy-4-hydroxybenzaldehyde (ethyl vanillin)
3-Ethoxy-4-hydroxybenzaldehyde
4-Hydroxy-3-ethoxybenzaldehyde
Benzaldehyde, 3-ethoxy-4-hydroxy-
Bourbonal
Ethavan
Ethovan
Ethylprotal
Ethylprotocatechualdehyde-3-ethyl ether
Ethylprotocatechuc aldehyde
NSC 1803
Protocatechuic aldehyde 3-ethyl ether
Protocatechuic aldehyde ethyl ether
Quantrovanil
Rhodiarome
Vanbeenol
Vanilal
Vanillal
Vanillin, ethyl-
Vanirom

Inchi: InChI=1S/C9H10O3/c1-2-12-9-5-7(6-10)3-4-8(9)11/h3-6,11H,2H2,1H3

InchiKey: CBOQJANXLMLOSS-UHFFFAOYSA-N

Formula: C9H10O3

SMILES: CCOc1cc(C=O)ccc1O

Mol. weight [g/mol]: 166.17

CAS: 121-32-4

Physical Properties

Property code	Value	Unit	Source
gf	-231.46	kJ/mol	Joback Method
hf	-399.14	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Influence of the aromatic ring substituents on phase equilibria of vanillins in binary systems with CO ₂
hvap	60.71	kJ/mol	Joback Method

log10ws	-1.77		Aqueous Solubility Prediction Method
logp	1.603		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1452.00		NIST Webbook
ripol	2414.00		NIST Webbook
ripol	2514.00		NIST Webbook
ripol	2514.00		NIST Webbook
tb	588.68	K	Joback Method
tc	812.18	K	Joback Method
tf	350.40	K	Aqueous Solubility Prediction Method
tf	352.98	K	Solid-liquid phase equilibrium and dissolution properties of ethyl vanillin in pure solvents
tf	351.00	K	Determination and Correlation of Ethyl Vanillin Solubility in Different Binary Solvents at Temperatures from 273.15 to 313.15 K
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.26	J/mol×K	588.68	Joback Method
cpg	314.95	J/mol×K	625.93	Joback Method
cpg	324.97	J/mol×K	663.18	Joback Method
cpg	334.37	J/mol×K	700.43	Joback Method
cpg	343.20	J/mol×K	737.68	Joback Method
cpg	351.51	J/mol×K	774.93	Joback Method
cpg	359.35	J/mol×K	812.18	Joback Method
dvisc	0.0004525	Paxs	436.51	Joback Method
dvisc	0.0008942	Paxs	406.08	Joback Method
dvisc	0.0002502	Paxs	466.95	Joback Method
dvisc	0.0001488	Paxs	497.38	Joback Method

dvisc	0.0000939	Paxs	527.81	Joback Method
dvisc	0.0000623	Paxs	558.25	Joback Method
dvisc	0.0000432	Paxs	588.68	Joback Method
hfust	23.10	kJ/mol	349.80	NIST Webbook
hsubt	101.50	kJ/mol	317.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{\text{vp}}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.75341e+02
Coeff. B	-1.86800e+04
Coeff. C	-2.20762e+01
Coeff. D	6.79415e-06
Temperature range (K), min.	350.65
Temperature range (K), max.	748.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1250.mol
Solid-liquid phase equilibrium and dissolution properties of ethyl vanillin in pure solvents:	https://www.doi.org/10.1016/j.jct.2016.10.029
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1250
Influence of the aromatic ring substituents on phase equilibria of NIST Webbook systems with CO₂:	https://www.doi.org/10.1016/j.fluid.2004.12.012
Joback Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121324&Units=SI
Aqueous Solubility Prediction Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Determination and Correlation of Ethyl Vanillin Solubility in Different Binary Vapour-Liquid Temperature Systems of 2-Ethoxy-3-hydroxybenzaldehyde in Acetone:	http://link.springer.com/article/10.1007/BF02311772
Method:	https://www.doi.org/10.1021/acs.jced.6b00972
	https://www.doi.org/10.1021/je700316s
	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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