3-ETHOXY-4-HYDROXYBENZALDEHYDE

Other names:	2-ethoxy-4-formylphenol
	3-Ethoxy-4-hydroxybenzadehyde (ethyl vanillin)
	4-hydroxy-3-ethoxybenzaldehyde
	Bourbonal
	Ethavan
	Ethovan
	Ethylprotal
	Ethylprotocatechualdehyde-3-ethyl ether
	Ethylprotocatechuic aldehyde
	NSC 1803
	Protocatechuic aldehyde 3-ethyl ether
	Protocatechuic aldehyde ethyl ether
	Quantrovanil
	Rhodiarome
	Vanbeenol
	Vanilal
	Vanillin, ethyl-
	Vanirom
	benzaldehyde, 3-ethoxy-4-hydroxy-
	ethyl vanillin
	vanillal
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]:	166.18
CAS:	121-32-4

Physical Properties

Property code	Value	Unit	Source
hfus	25.34	kJ/mol	Influence of the aromatic ring substituents on phase equilibria of vanillins in binary systems with CO2
hvap	73.05	kJ/mol	Cheméo Relay (1.0)
log10ws	-1.77		Aqueous Solubility Prediction Method
logp	1.603		Crippen Method

mcvol	127.220	ml/mol	McGowan Method
rinpol	1448.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1433.00		NIST Webbook
ripol	2514.00		NIST Webbook
ripol	2414.00		NIST Webbook
tb	546.13	K	Cheméo Relay (1.0)
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
tf	350.40	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.35	J/mol×K	812.18	Joback Method
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
dvisc	0.0008942	Pa×s	406.08	Joback Method
dvisc	0.0004525	Pa×s	436.51	Joback Method
dvisc	0.0002502	Pa×s	466.95	Joback Method
dvisc	0.0001488	Pa×s	497.38	Joback Method
dvisc	0.0000939	Pa×s	527.81	Joback Method
dvisc	0.0000623	Pa×s	558.25	Joback Method
dvisc	0.0000432	Pa×s	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(Pvp) = 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

Influence of the aromatic ring substituents on phase equilibria of vanillins in binary systems with CO2:	https://www.doi.org/10.1016/j.fluid.2004.12.012
Determination and Correlation of Ethyl Vanillin Solubility in Different Binary Solvents at Temperatures from 273.15 to 313.15 K:	https://www.doi.org/10.1021/acs.jced.6b00972
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1250
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Vapor-Liquid Equilibrium Behaviors of 3-Ethoxy-4-hydroxybenzaldehyde in Alcohol:	https://www.doi.org/10.1021/je700316s
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1250.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	
Solid-liquid phase equilibrium and dissolution properties of ethyl vanillin in pure solvents:	https://www.doi.org/10.1016/j.jct.2016.10.029
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121324&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0, beta):	
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point