Benzaldehyde, 3-ethoxy-2-hydroxy-

Other names:	3-Ethoxy-2-hydroxybenzaldehyde
	3-Ethoxy-2-hydroxybenzaldehye
	3-Ethoxysalicylaldehyde
	Novovanillin
	Salicylaldehyde, 3-ethoxy-
Inchi:	InChI=1S/C9H10O3/c1-2-12-8-5-3-4-7(6-10)9(8)11/h3-6,11H,2H2,1H3
InchiKey:	OFQBYHLLIJGMNP-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	CCOc1cccc(C=O)c1O
Mol. weight [g/mol]:	166.17
CAS:	492-88-6

Physical Properties

Property code	Value	Unit	Source
gf	-231.46	kJ/mol	Joback Method
hf	-399.14	kJ/mol	Joback Method
hfus	25.43	kJ/mol	Influence of the aromatic ring substituents on phase equilibria of vanillins in binary systems with CO2
hvap	60.71	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.603		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	588.68	K	Joback Method
tc	812.18	K	Joback Method
tf	406.08	K	Joback Method
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	0.0008942	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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C492886&Units=SI

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