Benzaldehyde, 2-hydroxy-3-methoxy-

Other names:	2-Hydroxy-3-methoxybenzaldehyde
	2-Hydroxy-m-anisaldehyde
	2-Vanillin
	3-Methoxy-2-hydroxybenzaldehyde
	3-Methoxysalicylaldehyde
	6-Formyl-2-methoxyphenol
	6-Formylguaiacol
	NSC 2150
	Ortho vanillin
	Orthovanilline
	Oxy-2 methoxy-3 benzaldehyde
	Vanillin
	m-Anisaldehyde, 2-hydroxy-
	o-Vanillin
	o-Vanilline
Inchi:	InChI=1S/C8H8O3/c1-11-7-4-2-3-6(5-9)8(7)10/h2-5,10H,1H3
InchiKey:	JJVNINGBHGBWJH-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	COc1cccc(C=O)c1O
Mol. weight [g/mol]:	152.15
CAS:	148-53-8

Physical Properties

Property code	Value	Unit	Source
gf	-239.88	kJ/mol	Joback Method
hf	-378.50	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Influence of the aromatic ring substituents on phase equilibria of vanillins in binary systems with CO2
hvap	58.48	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.213		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
rinpol	1367.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1330.50		NIST Webbook

rinpol	1367.00		NIST Webbook
tb	538.70	K	NIST Webbook
tc	793.56	K	Joback Method
tf	394.81	K	Joback Method
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	0.0010401	Pa×s	394.81	Joback Method
dvisc	0.0005373	Pa×s	423.31	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
hsubt	54.10	kJ/mol	292.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	401.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.59856e+01
Coeff. B	-5.20398e+03
Coeff. C	-1.00196e+02
Temperature range (K), min.	431.70
Temperature range (K), max.	587.73

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C148538&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
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
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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