Benzaldehyde, 3-hydroxy-4-methoxy-

Other names:	p-Anisaldehyde, 3-hydroxy-
	Isovanillin
	3-Hydroxy-p-anisaldehyde
	3-Hydroxy-4-methoxybenzaldehyde
	5-Formylguaiacol
	3-Hydroxy-para-anisaldehyde
	3-Hydroxyanisaldehyde
	Isovanilline
	Oxy-3 methoxy-4 benzaldehyde
Inchi:	InChI=1S/C8H8O3/c1-11-8-3-2-6(5-9)4-7(8)10/h2-5,10H,1H3
InchiKey:	JVTZFYYHCGSXJV-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	COc1ccc(C=O)cc1O
Mol. weight [g/mol]:	152.15
CAS:	621-59-0

Physical Properties

Property code	Value	Unit	Source
chs	-3838.00 ± 5.90	kJ/mol	NIST Webbook
gf	-239.88	kJ/mol	Joback Method
hf	-378.50	kJ/mol	Joback Method
hfus	19.39	kJ/mol	Joback Method
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	1401.00		NIST Webbook
rinpol	1468.60		NIST Webbook
tb	565.80	K	Joback Method
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	302.31	J/mol×K	755.60	Joback Method
cpg	294.87	J/mol×K	717.64	Joback Method
cpg	286.94	J/mol×K	679.68	Joback Method
cpg	278.48	J/mol×K	641.72	Joback Method
cpg	269.43	J/mol×K	603.76	Joback Method
cpg	309.32	J/mol×K	793.56	Joback Method
dvisc	0.0000536	Pa×s	565.80	Joback Method
dvisc	0.0000771	Pa×s	537.30	Joback Method
dvisc	0.0001155	Pa×s	508.80	Joback Method
dvisc	0.0001814	Pa×s	480.30	Joback Method
dvisc	0.0003017	Pa×s	451.81	Joback Method
dvisc	0.0005373	Pa×s	423.31	Joback Method
dvisc	0.0010401	Pa×s	394.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	452.20	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C621590&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
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
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