Benzaldehyde, 2,3-dimethoxy-

Other names:	o-Veratraldehyde
	2,3-Dimethoxybenzaldehyde
	2-Hydroxy-3-methoxybenzaldehyde, methyl ether
Inchi:	InChI=1S/C9H10O3/c1-11-8-5-3-4-7(6-10)9(8)12-2/h3-6H,1-2H3
InchiKey:	JIVGSHFYXPRRSZ-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1cccc(C=O)c1OC
Mol. weight [g/mol]:	166.17
CAS:	86-51-1

Physical Properties

Property code	Value	Unit	Source
gf	-191.47	kJ/mol	Joback Method
hf	-365.52	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	50.77	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.516		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	1391.50		NIST Webbook
rinpol	1391.50		NIST Webbook
rinpol	1362.00		NIST Webbook
tb	535.46	K	Joback Method
tc	746.40	K	Joback Method
tf	329.11	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.82	J/mol×K	535.46	Joback Method
cpg	331.68	J/mol×K	711.24	Joback Method
cpg	322.35	J/mol×K	676.09	Joback Method

cpg	312.49	J/mol×K	640.93	Joback Method
cpg	302.11	J/mol×K	605.77	Joback Method
cpg	291.21	J/mol×K	570.62	Joback Method
cpg	340.46	J/mol×K	746.40	Joback Method
dvisc	0.0001969	Pa×s	535.46	Joback Method
dvisc	0.0002394	Pa×s	501.07	Joback Method
dvisc	0.0002996	Pa×s	466.68	Joback Method
dvisc	0.0003887	Pa×s	432.29	Joback Method
dvisc	0.0005273	Pa×s	397.89	Joback Method
dvisc	0.0007578	Pa×s	363.50	Joback Method
dvisc	0.0011750	Pa×s	329.11	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.20	K	1.60	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86511&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
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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