3,4-Dimethoxy-5-hydroxybenzaldehyde

Other names: Benzaldehyde, 3-hydroxy-4,5-dimethoxy-
Inchi: InChI=1S/C9H10O4/c1-12-8-4-6(5-10)3-7(11)9(8)13-2/h3-5,11H,1-2H3
InchiKey: NVLTWXMZECWWPC-UHFFFAOYSA-N
Formula: C9H10O4
SMILES: COc1cc(C=O)cc(O)c1OC
Mol. weight [g/mol]: 182.17
CAS: 29865-90-5

Physical Properties

Property code	Value	Unit	Source
gf	-346.09	kJ/mol	Joback Method
hf	-542.83	kJ/mol	Joback Method
hfus	22.78	kJ/mol	Joback Method
hvap	63.78	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.222		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
tb	616.08	K	Joback Method
tc	837.67	K	Joback Method
tf	440.83	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.35	J/mol×K	616.08	Joback Method
cpg	335.72	J/mol×K	653.01	Joback Method
cpg	345.52	J/mol×K	689.94	Joback Method
cpg	354.78	J/mol×K	726.88	Joback Method
cpg	363.52	J/mol×K	763.81	Joback Method
cpg	371.79	J/mol×K	800.74	Joback Method
cpg	379.60	J/mol×K	837.67	Joback Method
dvisc	0.0003979	Pa×s	440.83	Joback Method

dvisc	0.0002252	Pa×s	470.04	Joback Method
dvisc	0.0001362	Pa×s	499.25	Joback Method
dvisc	0.0000871	Pa×s	528.45	Joback Method
dvisc	0.0000584	Pa×s	557.66	Joback Method
dvisc	0.0000407	Pa×s	586.87	Joback Method
dvisc	0.0000294	Pa×s	616.08	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	451.70	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=C29865905&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume