Ethanal, 2-(4-hydroxy-2,6-dimethoxyphenyl)

Inchi: InChI=1S/C9H10O4/c1-12-8-3-6(11)4-9(13-2)7(8)5-10/h3-5,11H,1-2H3
InchiKey: HZWPJAZIRZFCGX-UHFFFAOYSA-N
Formula: C9H10O4
SMILES: COc1cc(O)cc(OC)c1C=O
Mol. weight [g/mol]: 182.17

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
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook
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

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=R88457&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume