Homovanillin

Other names:	Ethanal, 2-(4-hydroxy-3-methoxyphenyl)
	2-(4-hydroxy-3-methoxyphenyl) acetaldehyde
	1-(4-Hydroxy-3-methoxyphenyl)-ethanal (homovanillin)
Inchi:	InChI=1S/C9H10O3/c1-12-9-6-7(4-5-10)2-3-8(9)11/h2-3,5-6,11H,4H2,1H3
InchiKey:	GOQGGGANVKPMNH-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1cc(CC=O)ccc1O
Mol. weight [g/mol]:	166.17
CAS:	5703-24-2

Physical Properties

Property code	Value	Unit	Source
gf	-231.46	kJ/mol	Joback Method
hf	-399.14	kJ/mol	Joback Method
hfus	21.98	kJ/mol	Joback Method
hvap	60.71	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.142		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	1406.00		NIST Webbook
rinpol	1406.00		NIST Webbook
tb	588.68	K	Joback Method
tc	812.18	K	Joback Method
tf	406.08	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.26	J/mol×K	588.68	Joback Method
cpg	351.51	J/mol×K	774.93	Joback Method
cpg	343.20	J/mol×K	737.68	Joback Method
cpg	334.37	J/mol×K	700.43	Joback Method

cpg	324.97	J/mol×K	663.18	Joback Method
cpg	314.95	J/mol×K	625.93	Joback Method
cpg	359.35	J/mol×K	812.18	Joback Method
dvisc	0.0000432	Pa×s	588.68	Joback Method
dvisc	0.0000623	Pa×s	558.25	Joback Method
dvisc	0.0000939	Pa×s	527.81	Joback Method
dvisc	0.0001488	Pa×s	497.38	Joback Method
dvisc	0.0002502	Pa×s	466.95	Joback Method
dvisc	0.0004525	Pa×s	436.51	Joback Method
dvisc	0.0008942	Pa×s	406.08	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5703242&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

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

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