Homovanillyl alcohol

Other names:	4-Hydroxy-3-methoxyphenylethyl alcohol
	4-Hydroxy-3-methoxyphenethyl alcohol
	Benzeneethanol, 4-hydroxy-3-methoxy-
	2-(4-Guaiacyl)-ethanol
	2-(4-Hydroxy-3-methoxyphenyl)-ethanol
	Guaiacyl ethanol
	Homovanillin alcohol
	Homovanilline alcohol
	4-(2-hydroxyethyl)guaiacol
Inchi:	InChI=1S/C9H12O3/c1-12-9-6-7(4-5-10)2-3-8(9)11/h2-3,6,10-11H,4-5H2,1H3
InchiKey:	XHUBSJRBOQIZNI-UHFFFAOYSA-N
Formula:	C9H12O3
SMILES:	COc1cc(CCO)ccc1O
Mol. weight [g/mol]:	168.19
CAS:	2380-78-1

Physical Properties

Property code	Value	Unit	Source
gf	-268.76	kJ/mol	Joback Method
hf	-465.79	kJ/mol	Joback Method
hfus	23.78	kJ/mol	Joback Method
hvap	70.67	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	0.936		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
rinpol	1542.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1534.00		NIST Webbook
ripol	2805.00		NIST Webbook
ripol	2802.00		NIST Webbook
ripol	2830.00		NIST Webbook
ripol	2830.00		NIST Webbook
ripol	2807.00		NIST Webbook
ripol	2786.00		NIST Webbook
tb	632.20	K	Joback Method

tc	837.13	K	Joback Method
tf	424.90	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.25	J/mol×K	632.20	Joback Method
cpg	346.25	J/mol×K	666.35	Joback Method
cpg	355.70	J/mol×K	700.51	Joback Method
cpg	364.64	J/mol×K	734.66	Joback Method
cpg	373.11	J/mol×K	768.82	Joback Method
cpg	381.17	J/mol×K	802.97	Joback Method
cpg	388.85	J/mol×K	837.13	Joback Method
dvisc	0.0006176	Pa×s	424.90	Joback Method
dvisc	0.0002336	Pa×s	459.45	Joback Method
dvisc	0.0001012	Pa×s	494.00	Joback Method
dvisc	0.0000489	Pa×s	528.55	Joback Method
dvisc	0.0000258	Pa×s	563.10	Joback Method
dvisc	0.0000147	Pa×s	597.65	Joback Method
dvisc	0.0000089	Pa×s	632.20	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2380781&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume