Phenol, 2-ethoxy-5-(1-propenyl)-

Other names:	1-Ethoxy-2-hydroxy-4-propenylbenzene
	Propenylguaethol
	trans-2-Ethoxy-5-(1-propenyl)phenol
	Hydroxy methyl anethol
	Isosafroeugenol
	Phenol, 2-ethoxy-5-propenyl-
	Vanitrope
	2-Ethoxy-5-propenylphenol
	6-Ethoxy-m-anol
	2-ethoxy-5-prop-1-enylphenol
Inchi:	InChI=1S/C11H14O2/c1-3-5-9-6-7-11(13-4-2)10(12)8-9/h3,5-8,12H,4H2,1-2H3/b5-3+
InchiKey:	RADIRXJQODWKGQ-HWKANZROSA-N
Formula:	C11H14O2
SMILES:	CC=Cc1ccc(OCC)c(O)c1
Mol. weight [g/mol]:	178.23
CAS:	94-86-0

Physical Properties

Property code	Value	Unit	Source
gf	-34.88	kJ/mol	Joback Method
hf	-237.62	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.824		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	589.94	K	Joback Method
tc	812.56	K	Joback Method
tf	381.54	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.75	J/mol×K	589.94	Joback Method
cpg	375.14	J/mol×K	627.04	Joback Method
cpg	387.68	J/mol×K	664.15	Joback Method
cpg	399.45	J/mol×K	701.25	Joback Method
cpg	410.54	J/mol×K	738.35	Joback Method
cpg	421.01	J/mol×K	775.46	Joback Method
cpg	430.94	J/mol×K	812.56	Joback Method
dvisc	0.0010233	Pa×s	381.54	Joback Method
dvisc	0.0004324	Pa×s	416.27	Joback Method
dvisc	0.0002086	Pa×s	451.01	Joback Method
dvisc	0.0001117	Pa×s	485.74	Joback Method
dvisc	0.0000650	Pa×s	520.47	Joback Method
dvisc	0.0000405	Pa×s	555.21	Joback Method
dvisc	0.0000267	Pa×s	589.94	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94860&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume