

Phenol, 2-methoxy-5-(1-propenyl)-, (E)-

Other names:	Phenol, 2-methoxy-5-propenyl-, (E)- trans-m-Propenyl guaiacol Isochavibetol
Inchi:	InChI=1S/C10H12O2/c1-3-4-8-5-6-10(12-2)9(11)7-8/h3-7,11H,1-2H3/b4-3+
InchiKey:	LHJZSWVADJCBNI-ONEGZZNKSA-N
Formula:	C10H12O2
SMILES:	CC=Cc1ccc(OC)c(O)c1
Mol. weight [g/mol]:	164.20
CAS:	19784-98-6

Physical Properties

Property code	Value	Unit	Source
gf	-43.30	kJ/mol	Joback Method
hf	-216.98	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.434		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
ripol	2312.00		NIST Webbook
ripol	2312.00		NIST Webbook
tb	567.06	K	Joback Method
tc	793.89	K	Joback Method
tf	370.27	K	Joback Method
vc	0.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.41	J/mol×K	567.06	Joback Method
cpg	327.96	J/mol×K	604.87	Joback Method
cpg	339.68	J/mol×K	642.67	Joback Method
cpg	350.65	J/mol×K	680.48	Joback Method

cpg	360.95	J/mol×K	718.28	Joback Method
cpg	370.65	J/mol×K	756.09	Joback Method
cpg	379.83	J/mol×K	793.89	Joback Method
dvisc	0.0012214	Paxs	370.27	Joback Method
dvisc	0.0005246	Paxs	403.07	Joback Method
dvisc	0.0002559	Paxs	435.87	Joback Method
dvisc	0.0001380	Paxs	468.67	Joback Method
dvisc	0.0000807	Paxs	501.46	Joback Method
dvisc	0.0000504	Paxs	534.26	Joback Method
dvisc	0.0000332	Paxs	567.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19784986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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