3-Allyl-6-methoxyphenol

Other names:	Phenol, 2-methoxy-5-(2-propenyl)-
	2-Methoxy-5-(2-propenyl)phenol
	Chavibetol
	Phenol, 5-allyl-2-methoxy-
	m-Eugenol
	Chavibetol (m-Eugenol)
	Chavibetol (2-Methoxy-5-(2-propenyl)phenol)
	5-Allyl-2-methoxyphenol
Inchi:	InChI=1S/C10H12O2/c1-3-4-8-5-6-10(12-2)9(11)7-8/h3,5-7,11H,1,4H2,2H3
InchiKey:	NPBVQXIMTZKSBA-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	C=CCc1ccc(OC)c(O)c1
Mol. weight [g/mol]:	164.20
CAS:	501-19-9

Physical Properties

Property code	Value	Unit	Source
gf	-35.68	kJ/mol	Joback Method
hf	-208.77	kJ/mol	Joback Method
hfus	21.00	kJ/mol	Joback Method
hvap	55.55	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.129		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1362.00		NIST Webbook
ripol	2217.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2217.00		NIST Webbook
tb	559.58	K	Joback Method
tc	781.19	K	Joback Method
tf	373.59	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.59	J/mol×K	781.19	Joback Method
cpg	370.45	J/mol×K	744.26	Joback Method
cpg	360.77	J/mol×K	707.32	Joback Method
cpg	350.49	J/mol×K	670.39	Joback Method
cpg	339.55	J/mol×K	633.45	Joback Method
cpg	327.88	J/mol×K	596.52	Joback Method
cpg	315.44	J/mol×K	559.58	Joback Method
dvisc	0.0012460	Pa×s	373.59	Joback Method
dvisc	0.0000422	Pa×s	559.58	Joback Method
dvisc	0.0000629	Pa×s	528.58	Joback Method
dvisc	0.0000985	Pa×s	497.58	Joback Method
dvisc	0.0001637	Pa×s	466.59	Joback Method
dvisc	0.0002925	Pa×s	435.59	Joback Method
dvisc	0.0005711	Pa×s	404.59	Joback Method
hvapt	61.40	kJ/mol	436.00	NIST Webbook

Sources

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=C501199&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
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