

Phenol, 2-methoxy-3-(2-propenyl)-

Other names:	3-Allylguaiacol
Inchi:	InChI=1S/C10H12O2/c1-3-5-8-6-4-7-9(11)10(8)12-2/h3-4,6-7,11H,1,5H2,2H3
InchiKey:	HKHVWTUGAJEQNP-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	C=CCc1cccc(O)c1OC
Mol. weight [g/mol]:	164.20
CAS:	1941-12-4

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	1362.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	559.58	K	Joback Method
tc	781.19	K	Joback Method
tf	373.59	K	Joback Method
vc	0.453	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.44	J/mol×K	559.58	Joback Method
cpg	327.88	J/mol×K	596.52	Joback Method
cpg	339.55	J/mol×K	633.45	Joback Method
cpg	350.49	J/mol×K	670.39	Joback Method
cpg	360.77	J/mol×K	707.32	Joback Method

cpg	370.45	J/molxK	744.26	Joback Method
cpg	379.59	J/molxK	781.19	Joback Method
dvisc	0.0012460	Paxs	373.59	Joback Method
dvisc	0.0005711	Paxs	404.59	Joback Method
dvisc	0.0002925	Paxs	435.59	Joback Method
dvisc	0.0001637	Paxs	466.59	Joback Method
dvisc	0.0000985	Paxs	497.58	Joback Method
dvisc	0.0000629	Paxs	528.58	Joback Method
dvisc	0.0000422	Paxs	559.58	Joback Method

Sources

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=C1941124&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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