trans-Isoeugenol

Other names:	(E)-2-Methoxy-4-(prop-1-enyl)phenol
	(E)-2-methoxy-4-(prop-1-en-1-yl)phenol
	(E)-isoeugenol
	2-methoxy-4-(1E)-1-propen-1-yl-phenol
	4-(1-Propenyl)-2-methoxyphenol
	4-(1-Propenyl)-2-methoxyphenol (trans-isoeugenol)
	E-4-Propenyl-2-methoxyphenol
	Isoeugenol E
	NSC 209522
	Phenol, 2-methoxy-4-(1-propenyl)-, (E)-
	Phenol, 2-methoxy-4-propenyl-, (E)-
	iso-Eugenol 2
	trans-2-Methoxy-4-(1-propenyl)phenol
	trans-2-Methoxy-4-propenylphenol
	trans-p-Propenylquaiacol
Inchi:	InChI=1S/C10H12O2/c1-3-4-8-5-6-9(11)10(7-8)12-2/h3-7,11H,1-2H3/b4-3+
InchiKey:	BJIOGJUNALELMI-ONEGZZNKSA-N
Formula:	C10H12O2
SMILES:	CC=Cc1ccc(O)c(OC)c1
Mol. weight [g/mol]:	164.20
CAS:	5932-68-3

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
rinpol	1474.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1459.00		NIST Webbook

rinpol	1411.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1436.40		NIST Webbook
rinpol	1436.40		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1458.40		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1455.00		NIST Webbook
ripol	2355.00		NIST Webbook
ripol	2309.00		NIST Webbook
ripol	2394.00		NIST Webbook
ripol	2347.00		NIST Webbook
ripol	2352.00		NIST Webbook
ripol	2352.00		NIST Webbook
ripol	2339.00		NIST Webbook
ripol	2314.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2368.00		NIST Webbook
ripol	2372.00		NIST Webbook
ripol	2383.00		NIST Webbook
tb	567.06	K	Joback Method
tc	793.89	K	Joback Method
tf	370.27	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.83	J/mol×K	793.89	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	315.41	J/mol×K	567.06	Joback Method
dvisc	0.0000504	Pa×s	534.26	Joback Method
dvisc	0.0000807	Pa×s	501.46	Joback Method
dvisc	0.0001380	Pa×s	468.67	Joback Method
dvisc	0.0002559	Pa×s	435.87	Joback Method
dvisc	0.0005246	Pa×s	403.07	Joback Method
dvisc	0.0000332	Pa×s	567.06	Joback Method
dvisc	0.0012214	Pa×s	370.27	Joback Method
hvapt	69.10	kJ/mol	391.50	NIST Webbook
pvap	6.57e-03	kPa	325.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	9.75e-03	kPa	330.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	5.61e-03	kPa	323.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.02	kPa	336.30	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.02	kPa	338.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.02	kPa	340.20	Vaporization thermodynamics of compounds modeling lignin structural units

pvap	0.03	kPa	343.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.03	kPa	345.10	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.04	kPa	348.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.04	kPa	350.10	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.05	kPa	353.10	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.06	kPa	356.10	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.07	kPa	358.10	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	4.49e-03	kPa	320.30	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	3.71e-03	kPa	318.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	3.13e-03	kPa	316.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	2.89e-03	kPa	315.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	2.41e-03	kPa	313.20	Vaporization thermodynamics of compounds modeling lignin structural units

pvap	8.38e-03	kPa	328.10	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.01	kPa	333.20	Vaporization thermodynamics of compounds modeling lignin structural units

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vaporization thermodynamics of compounds modeling lignin structural units:	https://www.doi.org/10.1016/j.fluid.2019.03.004
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=C5932683&Units=SI

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
pvap:	Vapor 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