2-Methoxy-4-(1-propenyl)phenol (isoeugenol)

Other names:	1-(3-Methoxy-4-hydroxyphenyl)-1-propene
	1-Hydroxy-2-methoxy-4-propenylbenzene
	2-Methoxy-4-(1-propenyl)phenol
	2-Methoxy-4-propenylphenol
	2-Methoxy-4-propenylphenol (isoeugenol)
	3-Methoxy-4-hydroxy-1-propenylbenzene
	4-(1-Propenyl)-2-methoxyphenol (cis-isoeugenol)
	4-Hydroxy-3-methoxy-1-propenylbenzene
	4-Hydroxy-3-methoxypropenylbenzene
	4-Propenylguaiacol
	Isoeugenol
	Isoeugenol (I)
	Isoeugenol (II)
	Isoeugenol,c&t
	NCI-C60979
	NSC 6769
	Phenol, 2-methoxy-4-(1-propen-1-yl)-
	Phenol, 2-methoxy-4-propenyl-
	Propenyl guaiacol
	o-Eugenol, isomer
Inchi:	InChI=1S/C10H12O2/c1-3-4-8-5-6-9(11)10(7-8)12-2/h3-7,11H,1-2H3
InchiKey:	BJIOGJUNALELMI-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC=Cc1ccc(O)c(OC)c1
Mol. weight [g/mol]:	164.20
CAS:	97-54-1

Physical Properties

Property code	Value	Unit	Source
hf	-199.86	kJ/mol	Cheméo Relay (1.0)
hfus	22.48	kJ/mol	Joback Method
hvap	73.89	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.41		Cheméo Relay (1.0)
logp	2.434		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
rinpol	1402.00		NIST Webbook
rinpol	1451.00		NIST Webbook

rinpol	1447.00	NIST Webbook
rinpol	1459.40	NIST Webbook
rinpol	1448.00	NIST Webbook
rinpol	1397.00	NIST Webbook
rinpol	1428.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1403.00	NIST Webbook
rinpol	1451.00	NIST Webbook
rinpol	1452.00	NIST Webbook
rinpol	1468.00	NIST Webbook
rinpol	1465.00	NIST Webbook
rinpol	1466.00	NIST Webbook
rinpol	1468.00	NIST Webbook
rinpol	1474.00	NIST Webbook
rinpol	1471.00	NIST Webbook
rinpol	1452.00	NIST Webbook
rinpol	1404.00	NIST Webbook
rinpol	1436.00	NIST Webbook
rinpol	1415.00	NIST Webbook
rinpol	1396.00	NIST Webbook
rinpol	1457.00	NIST Webbook
rinpol	1405.00	NIST Webbook
rinpol	1430.00	NIST Webbook
rinpol	1403.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1429.00	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1427.00	NIST Webbook
rinpol	1428.00	NIST Webbook
rinpol	1408.00	NIST Webbook
rinpol	1451.00	NIST Webbook
rinpol	1404.00	NIST Webbook
rinpol	1436.30	NIST Webbook
rinpol	1460.00	NIST Webbook
rinpol	1414.80	NIST Webbook
rinpol	1456.00	NIST Webbook
rinpol	1454.00	NIST Webbook
rinpol	1422.00	NIST Webbook
rinpol	1460.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1403.00	NIST Webbook
rinpol	1436.30	NIST Webbook

ripol	2266.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2356.00		NIST Webbook
ripol	2352.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2268.00		NIST Webbook
ripol	2322.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2332.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2279.00		NIST Webbook
ripol	2338.00		NIST Webbook
ripol	2319.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2336.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2308.00		NIST Webbook
ripol	2304.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2299.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2326.00		NIST Webbook
ripol	2338.00		NIST Webbook
ripol	2271.00		NIST Webbook
tb	526.65 ± 2.00	K	NIST Webbook
tf	355.05	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.65	J/mol×K	756.09	Joback Method
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	315.41	J/mol×K	567.06	Joback Method
dvisc	0.0002559	Pa×s	435.87	Joback Method
dvisc	0.0005246	Pa×s	403.07	Joback Method
dvisc	0.0012214	Pa×s	370.27	Joback Method

dvisc	0.0001380	Pa×s	468.67	Joback Method
dvisc	0.0000807	Pa×s	501.46	Joback Method
dvisc	0.0000504	Pa×s	534.26	Joback Method
dvisc	0.0000332	Pa×s	567.06	Joback Method
hvapt	60.70	kJ/mol	449.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.80200e+01
Coeff. B	-7.68048e+03
Coeff. C	2.82770e+01
Temperature range (K), min.	398.15
Temperature range (K), max.	576.08

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97541&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point