Methyleugenol

Other names:	1,2-dimethoxy-4-(2-propenyl)benzene
	1,2-dimethoxy-4-allylbenzene
	1,3,4-Eugenol methyl ether
	1-(3,4-Dimethoxyphenyl)-2-propene
	1-Allyl-3,4-dimethoxybenzene
	3,4-Dimethoxyallylbenzene
	4-Allyl-1,2-dimethoxybenzene
	4-Allyl-1,2-dimethyoxybenzene
	4-Allylveratrole
	Benzene, 1,2-dimethoxy-4-(2-propen-1-yl)-
	Benzene, 1,2-dimethoxy-4-(2-propenyl)-
	Benzene, 4-(2-propenyl)-1,2-dimethoxy
	Benzene, 4-allyl-1,2-dimethoxy-
	Ent 21040
	Eugenol methyl
	Eugenol methyl ether
	Eugenyl methyl ether
	Methyl eugenol ether
	Methyl eugenyl ether
	NSC 209528
	O-Methyleugenol
	Veratrole methyl ether
	o-Methyl eugenol ether
Inchi:	InChI=1S/C11H14O2/c1-4-5-9-6-7-10(12-2)11(8-9)13-3/h4,6-8H,1,5H2,2-3H3
InchiKey:	ZYEMGPIYFIJGTP-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	C=CCc1ccc(OC)c(OC)c1
Mol. weight [g/mol]:	178.23
CAS:	93-15-2

Physical Properties

Property code	Value	Unit	Source
gf	12.73	kJ/mol	Joback Method
hf	-195.79	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	47.83	kJ/mol	Joback Method

log10ws	-2.79		Crippen Method
logp	2.432		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1400.00		NIST Webbook
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tb	527.90	K	NIST Webbook
tc	734.40	K	Joback Method
tf	307.89	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.58	J/mol×K	529.24	Joback Method
cpg	346.58	J/mol×K	563.43	Joback Method
cpg	359.96	J/mol×K	597.63	Joback Method
cpg	372.71	J/mol×K	631.82	Joback Method
cpg	384.84	J/mol×K	666.01	Joback Method
cpg	396.35	J/mol×K	700.21	Joback Method
cpg	407.24	J/mol×K	734.40	Joback Method
dvisc	0.0010599	Pa×s	307.89	Joback Method
dvisc	0.0006390	Pa×s	344.78	Joback Method
dvisc	0.0004248	Pa×s	381.67	Joback Method
dvisc	0.0003035	Pa×s	418.56	Joback Method
dvisc	0.0002290	Pa×s	455.46	Joback Method
dvisc	0.0001802	Pa×s	492.35	Joback Method
dvisc	0.0001466	Pa×s	529.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.00 ± 1.00	K	1.30	NIST Webbook

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	100.00	1031.0

Reference *https://www.doi.org/10.1021/acs.jced.8b00939*

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=C93152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Physical Properties of Model and Real Systems Composed of Essential Oils and Hydroalcoholic Solvents at 298.2 K and Atmospheric Pressure:	https://www.doi.org/10.1021/acs.jced.8b00939

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
rhol:	Liquid Density
rinpol:	Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume