

Eugenol

Other names:

1,3,4-Eugenol
1-Hydroxy-2-methoxy-4-allylbenzene
1-Hydroxy-2-methoxy-4-prop-2-enylbenzene
2-Hydroxy-5-allylanisole
2-Methoxy-1-hydroxy-4-allylbenzene
2-Methoxy-4-(2-propenyl)phenol
2-Methoxy-4-allylphenol
2-Methoxy-4-prop-2-enylphenol
2-Metoksy-4-allilofenol
4-(2-Propenyl)-2-methoxyphenol
4-(2-Propenyl)-2-methoxyphenol (eugenol)
4-Allyl-1-hydroxy-2-methoxybenzene
4-Allyl-2-methoxyphenol
4-Allyl-2-methoxyphenol (eugenol)
4-Allylcatechol-2-methyl ether
4-Allylguaiacol
4-Hydroxy-3-methoxyallylbenzene
4-allyl-2-methoxyphenol (eugenol)
4-hydroxy-3-methoxy-1-allylbenzene
Allylguaiacol
Caryophyllic acid
Engenol
Eugenic acid
Eugenol (2-Methoxy-4-(2-propenyl)phenol)
FA 100
FEMA No. 2467
NCI-C50453
NSC 209525
Phenol, 2-methoxy-4-(2-propen-1-yl)-
Phenol, 2-methoxy-4-(2-propenyl)-
Phenol, 4-allyl-2-methoxy-
p-Allylguaiacol
p-Eugenol

Inchi: InChI=1S/C10H12O2/c1-3-4-8-5-6-9(11)10(7-8)12-2/h3,5-7,11H,1,4H2,2H3

InchiKey: RRAFCDWBNXTKKO-UHFFFAOYSA-N

Formula: C10H12O2

SMILES: C=CCc1ccc(O)c(OC)c1

Mol. weight [g/mol]: 164.20

CAS: 97-53-0

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	66.30	kJ/mol	NIST Webbook
log10ws	-1.56		Estimated Solubility Method
log10ws	-1.56		Aqueous Solubility Prediction Method
logp	2.129		Crippen Method
mccvol	135.440	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
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tb	526.40	K	NIST Webbook
tb	526.65 ± 1.50	K	NIST Webbook
tc	781.19	K	Joback Method
tf	263.78	K	Aqueous Solubility Prediction Method

vc	0.453	m3/kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.59	J/mol×K	781.19	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
cpg	370.45	J/mol×K	744.26	Joback Method
cpl	343.20	J/mol×K	293.00	NIST Webbook
dvisc	0.0001637	Pa×s	466.59	Joback Method
dvisc	0.0002925	Pa×s	435.59	Joback Method
dvisc	0.0000985	Pa×s	497.58	Joback Method
dvisc	0.0012460	Pa×s	373.59	Joback Method
dvisc	0.0000629	Pa×s	528.58	Joback Method
dvisc	0.0000422	Pa×s	559.58	Joback Method
dvisc	0.0005711	Pa×s	404.59	Joback Method
hvapt	57.70	kJ/mol	461.00	NIST Webbook
hvapt	66.10	kJ/mol	309.00	NIST Webbook
hvapt	60.30	kJ/mol	438.50	NIST Webbook
pvap	3.90e-04	kPa	283.70	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	6.60e-04	kPa	289.00	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	1.11e-03	kPa	293.90	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	2.87e-03	kPa	303.70	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	4.47e-03	kPa	308.70	Vaporization thermodynamics of compounds modeling lignin structural units

pvap	7.09e-03	kPa	313.70	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.01	kPa	318.90	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.02	kPa	323.60	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.02	kPa	328.60	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.03	kPa	333.60	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.05	kPa	338.50	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.07	kPa	343.50	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	3.00e-04	kPa	281.10	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	1.79e-03	kPa	298.90	Vaporization thermodynamics of compounds modeling lignin structural units
rfi	1.54070		293.15	Solubility of hydrogen in bio-oil compounds
rhoI	1022.15	kg/m3	343.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model

rhoI	1026.60	kg/m3	338.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1031.04	kg/m3	333.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1035.48	kg/m3	328.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1039.92	kg/m3	323.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1044.35	kg/m3	318.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1048.78	kg/m3	313.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1053.21	kg/m3	308.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model

rhoI	1057.64	kg/m3	303.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1062.06	kg/m3	298.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1066.48	kg/m3	293.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1070.90	kg/m3	288.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.71278e+01
Coeff. B	-6.37215e+03
Coeff. C	-1.70150e+01
Temperature range (K), min.	395.40
Temperature range (K), max.	556.28

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	100.00	1062.0
Reference		https://www.doi.org/10.1021/acs.jced.8b00939

Sources

Vaporization thermodynamics of compounds modeling lignin structural	https://www.doi.org/10.1016/j.fluid.2019.03.004
Solubility of hydrogen in bio-oil compounds:	https://www.doi.org/10.1016/j.jct.2016.07.010
Physical Properties of Model and Real Systems Composed of Essential Oils and Hydroalcoholic Solvents at 298.2 K	https://www.doi.org/10.1021/acs.jced.8b00939
NIST Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97530&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Limiting Diffusion Coefficients of Ethyl Benzoate, Benzylacetone, and Eugenol	https://www.doi.org/10.1021/je700646e
Experimental Densities, Superheated Vapor Densities, and Speed of Sound of Substituted Phenols and Their Equilibrium with the Primary	https://www.doi.org/10.1021/je4003256
Flory-Huggins Model: Ternary Phase Diagrams for the Carbon Dioxide + dichloromethane + Eugenol and Quaternary systems	https://www.doi.org/10.1016/j.jct.2015.08.016
The Yaws Handbook of Vapor Pressure:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
rfi:	Refractive Index
rhof:	Liquid Density
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

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