

Benzene, 1,2-dimethoxy-4-(2-propenyl)-

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-dimethoxybenzene 4-Allylveratrole Benzene, 1,2-dimethoxy-4-(2-propen-1-yl)- 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 methyleugenol 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

Physical Properties

Property code	Value	Unit	Source
hfus	18.61	kJ/mol	Joback Method
hvap	67.46	kJ/mol	Cheméo Relay (1.0)
ie	7.87	eV	Cheméo Relay (1.0)
log10ws	-2.79		Cheméo Relay (1.0)
logp	2.432		Crippen Method

mcvol	149.530	ml/mol	McGowan Method
rinpol	1371.00		NIST Webbook
rinpol	1374.00		NIST Webbook
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ripol	1962.00		NIST Webbook
tb	527.90	K	NIST Webbook
tf	286.72	K	Cheméo Relay (1.0)

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93152&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):	
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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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