

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

Other names:	Benzene, 1,2-dimethoxy-4-propenyl- Isoeugenol methyl ether Isoeugenyl methyl ether Isohomogenol Methylisoeugenol O-Methylisoeugenol 1-(3,4-Dimethoxyphenyl)-1-propene 1-Veratryl-1-propene 3,4-Dimethoxypropenylbenzene 4-Propenyl-1,2-dimethoxybenzene 4-Propenylveratrole 1-Propene, 1-(3,4-dimethoxyphenyl)- 1,3,4-Isoeugenol methyl ether Benzene, 4-(1-propenyl)-1,2-dimethoxy Isomethyleugenol Benzene, 1,2-dimethoxy-4-(1-propen-1-yl)- NSC 46111 Veratrole, 4-propenyl- 1,2-Dimethoxy-4-(1-propenyl)-benzene 4-prop-1-enylveratrole
Inchi:	InChI=1S/C11H14O2/c1-4-5-9-6-7-10(12-2)11(8-9)13-3/h4-8H,1-3H3
InchiKey:	NNWHUJCUHAELCL-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	<chem>CC=Cc1ccc(OC)c(OC)c1</chem>
Mol. weight [g/mol]:	178.23
CAS:	93-16-3

Physical Properties

Property code	Value	Unit	Source
gf	5.11	kJ/mol	Joback Method
hf	-204.00	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	48.46	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.737		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method

rinpol	1492.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1504.00		NIST Webbook
ripol	2194.00		NIST Webbook
ripol	2189.00		NIST Webbook
ripol	2196.00		NIST Webbook
ripol	2126.00		NIST Webbook
ripol	2185.00		NIST Webbook
ripol	2176.00		NIST Webbook
tb	536.20	K	NIST Webbook
tc	746.85	K	Joback Method
tf	304.57	K	Joback Method
vc	0.559	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.08	J/mol×K	536.72	Joback Method
cpg	347.28	J/mol×K	571.74	Joback Method
cpg	360.80	J/mol×K	606.76	Joback Method
cpg	373.65	J/mol×K	641.78	Joback Method
cpg	385.84	J/mol×K	676.80	Joback Method
cpg	397.38	J/mol×K	711.82	Joback Method
cpg	408.27	J/mol×K	746.85	Joback Method

dvisc	0.0010229	Paxs	304.57	Joback Method
dvisc	0.0005877	Paxs	343.26	Joback Method
dvisc	0.0003778	Paxs	381.95	Joback Method
dvisc	0.0002634	Paxs	420.64	Joback Method
dvisc	0.0001952	Paxs	459.34	Joback Method
dvisc	0.0001515	Paxs	498.03	Joback Method
dvisc	0.0001220	Paxs	536.72	Joback Method
hvapt	61.90	kJ/mol	439.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C93163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ripol:	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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