Estragole

Other names:	1-Allyl-4-methoxybenzene
	1-Methoxy-4-(2-propenyl)benzene
	1-methoxy-4-prop-2-enylbenzene
	3-(p-Methoxyphenyl)propene
	4-Allyl-1-methoxybenzene
	4-Allylanisole
	4-Allylmethoxybenzene
	4-Methoxyallylbenzene
	Anisole, p-allyl-
	Benzene, 1-methoxy, 4-prop-2-enyl
	Benzene, 1-methoxy-4-(2-propen-1-yl)-
	Benzene, 1-methoxy-4-(2-propenyl)-
	Chavicol methyl ether
	Chavicol, O-methyl-
	Chavicol, methyl-
	Chavicyl methyl ether
	Esdragol
	Esdragole
	Esdragon
	Estragol
	Estragol (Methylchavicol)
	Ether, p-allylphenyl methyl
	Isoanethole
	Methyl chavicol
	Methyl chavicole
	NCI-C60946
	NSC 404113
	Tarragon
	methyl chavicole (estragole)
	p-Allylanisole
	p-Allylmethoxybenzene
	p-Allylphenyl methyl ether
	p-Methoxyallylbenzene
	para-Allylanisole
	para-Allylanisole (estragole)
Inchi:	InChI=1S/C10H12O/c1-3-4-9-5-7-10(11-2)8-6-9/h3,5-8H,1,4H2,2H3
InchiKey:	ZFMSMUAANRJZFM-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	C=CCc1ccc(OC)cc1
Mol. weight [g/mol]:	148.20

CAS: 140-67-0

Physical Properties

Property code	Value	Unit	Source
gf	118.94	kJ/mol	Joback Method
hf	-31.46	kJ/mol	Joback Method
hfus	15.22	kJ/mol	Joback Method
hvap	42.53	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
log10ws	-2.92		Aqueous Solubility Prediction Method
log10ws	-2.92		Estimated Solubility Method
logp	2.424		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	1158.00		NIST Webbook
rinpol	1180.70		NIST Webbook
rinpol	1180.70		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1195.00		NIST Webbook
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ripol	1685.00		NIST Webbook
tb	488.70	K	NIST Webbook
tb	493.00	K	NIST Webbook
tb	488.65 ± 3.00	K	NIST Webbook
tc	687.84	K	Joback Method
tf	261.87	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.98	J/mol×K	687.84	Joback Method
cpg	277.93	J/mol×K	513.77	Joback Method
cpg	290.86	J/mol×K	548.59	Joback Method
cpg	303.11	J/mol×K	583.40	Joback Method
cpg	314.70	J/mol×K	618.21	Joback Method
cpg	325.65	J/mol×K	653.02	Joback Method
cpg	264.30	J/mol×K	478.96	Joback Method
dvisc	0.0017608	Pa×s	261.87	Joback Method
dvisc	0.0009678	Pa×s	298.05	Joback Method
dvisc	0.0006055	Pa×s	334.23	Joback Method
dvisc	0.0004152	Pa×s	370.41	Joback Method
dvisc	0.0003045	Pa×s	406.60	Joback Method
dvisc	0.0001884	Pa×s	478.96	Joback Method
dvisc	0.0002349	Pa×s	442.78	Joback Method
hvapt	56.30	kJ/mol	406.50	NIST Webbook
pvap	3.78e-03	kPa	279.10	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	5.83e-03	kPa	284.10	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	9.12e-03	kPa	288.90	Vaporization thermodynamics of compounds modeling lignin structural units

pvap	0.01	kPa	293.80	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.02	kPa	298.80	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.03	kPa	303.70	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.05	kPa	308.80	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.07	kPa	313.70	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.09	kPa	318.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.13	kPa	323.20	Vaporization thermodynamics of compounds modeling lignin structural units

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60453e+01
Coeff. B	-5.05630e+03
Coeff. C	-4.62110e+01
Temperature range (K), min.	367.09
Temperature range (K), max.	517.27

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vaporization thermodynamics of compounds modeling lignin structural units:	https://www.doi.org/10.1016/j.fluid.2019.03.004
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C140670&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
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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