

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

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-Allylmethoxybenzene 4-allylanisole 4-methoxyallylbenzene Benzene, 1-methoxy, 4-prop-2-enyl Benzene, 1-methoxy-4-(2-propen-1-yl)- Chavicol methyl ether Chavicol, methyl- Chavicyl methyl ether Esdragol Esdragole Esdragon Estragol Estragol (Methylchavicol) Ether, p-allylphenyl methyl Methyl chavicole NCI-C60946 NSC 404113 Tarragon anisole, p-allyl- chavicol, O-methyl- estragole isoanethole methyl chavicol methyl chavicole (estragole) p-Allylanisole p-Allylmethoxybenzene p-Methoxyallylbenzene p-allylphenyl methyl ether 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:	<chem>C=CCc1ccc(OC)cc1</chem>
Mol. weight [g/mol]:	148.21

Physical Properties

Property code	Value	Unit	Source
hfus	15.22	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	NIST Webbook
log10ws	-2.92		Estimated Solubility Method
log10ws	-2.92		Aqueous Solubility Prediction Method
logp	2.424		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
rinpol	1175.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1181.00		NIST Webbook
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rinpol	1179.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1201.00		NIST Webbook
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tb	488.65 ± 3.00	K	NIST Webbook
tb	493.00	K	NIST Webbook
tb	488.70	K	NIST Webbook
tc	686.92	K	Cheméo Relay (1.0)
tf	248.79	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.30	J/mol×K	478.96	Joback Method
cpg	335.98	J/mol×K	687.84	Joback Method
cpg	325.65	J/mol×K	653.02	Joback Method
cpg	314.70	J/mol×K	618.21	Joback Method
cpg	303.11	J/mol×K	583.40	Joback Method
cpg	290.86	J/mol×K	548.59	Joback Method
cpg	277.93	J/mol×K	513.77	Joback Method
dvisc	0.0001884	Pa×s	478.96	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	0.0002349	Pa×s	442.78	Joback Method
dvisc	0.0017608	Pa×s	261.87	Joback Method
hvapt	56.30	kJ/mol	406.50	NIST Webbook
pvap	0.03	kPa	303.70	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.13	kPa	323.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.09	kPa	318.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	3.78e-03	kPa	279.10	Vaporization thermodynamics of compounds modeling lignin structural units

pvap	0.07	kPa	313.70	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.05	kPa	308.80	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	5.83e-03	kPa	284.10	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.02	kPa	298.80	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.01	kPa	293.80	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	9.12e-03	kPa	288.90	Vaporization thermodynamics of compounds modeling lignin structural units

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C140670&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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

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