1,3-Benzodioxole, 4-methoxy-6-(2-propenyl)-

Other names:	4-Methoxy-6-(2-propenyl)-1,3-benzodioxole
	5-Allyl-1-methoxy-2,3-(methylenedioxy)benzene
	6-Allyl-4-methoxy-1,3-benzodioxole
	Benzene, 5-allyl-1-methoxy-2,3-(methylenedioxy)-
	Myristicin
	Myristicine
Inchi:	InChI=1S/C11H12O3/c1-3-4-8-5-9(12-2)11-10(6-8)13-7-14-11/h3,5-6H,1,4,7H2,2H3
InchiKey:	BNWJOHGLIBDBOB-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	C=CCc1cc(OC)c2c(c1)OCO2
Mol. weight [g/mol]:	192.21
CAS:	607-91-0

Physical Properties

Property code	Value	Unit	Source
gf	4.32	kJ/mol	Joback Method
hf	-245.90	kJ/mol	Joback Method
hfus	30.05	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.152		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1507.00		NIST Webbook

rinpol	1516.00	NIST Webbook
rinpol	1519.00	NIST Webbook
rinpol	1523.00	NIST Webbook
rinpol	1516.00	NIST Webbook
rinpol	1522.00	NIST Webbook
rinpol	1525.20	NIST Webbook
rinpol	1519.00	NIST Webbook
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rinpol	1563.00		NIST Webbook
ripol	2289.00		NIST Webbook
ripol	2296.00		NIST Webbook
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ripol	2272.00		NIST Webbook
ripol	2286.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2247.00		NIST Webbook
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ripol	2262.00		NIST Webbook
ripol	2257.00		NIST Webbook
ripol	2246.00		NIST Webbook
ripol	2258.00		NIST Webbook
ripol	2256.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2225.00		NIST Webbook
tb	577.11	K	Joback Method
tc	797.56	K	Joback Method

tf	373.50	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.05	J/mol×K	797.56	Joback Method
cpg	408.46	J/mol×K	760.81	Joback Method
cpg	398.23	J/mol×K	724.07	Joback Method
cpg	387.31	J/mol×K	687.33	Joback Method
cpg	375.67	J/mol×K	650.59	Joback Method
cpg	363.26	J/mol×K	613.85	Joback Method
cpg	350.04	J/mol×K	577.11	Joback Method
dvisc	0.0014201	Pa×s	373.50	Joback Method
dvisc	0.0003548	Pa×s	577.11	Joback Method
dvisc	0.0004159	Pa×s	543.17	Joback Method
dvisc	0.0004980	Pa×s	509.24	Joback Method
dvisc	0.0006118	Pa×s	475.31	Joback Method
dvisc	0.0007758	Pa×s	441.37	Joback Method
dvisc	0.0010235	Pa×s	407.44	Joback Method
hvapt	61.20	kJ/mol	460.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.76626e+01
Coeff. B	-7.04896e+03
Coeff. C	-9.26200e+00
Temperature range (K), min.	414.96
Temperature range (K), max.	579.98

Sources

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=C607910&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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