Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-

Other names:	Benzene, 5-allyl-1,2,3-trimethoxy-
	Elemicin
	3,4,5-Trimethoxyallylbenzene
	5-Allyl-1,2,3-trimethoxybenzene
	1,2,3-Trimethoxy-5-(2-propenyl)-benzene
	1,2,3-Trimethoxy-5-allylbenzene
	4-Allyl-1,2,6-trimethoxybenzene
	Benzene, 5-(2-propenyl)-1,2,3-trimethoxy
	Elemicine
	1,2,3-trimethoxy-5-allylbenzene (elemicin)
Inchi:	InChI=1S/C12H16O3/c1-5-6-9-7-10(13-2)12(15-4)11(8-9)14-3/h5,7-8H,1,6H2,2-4H3
InchiKey:	BPLQKQKXWHCZSS-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	C=CCc1cc(OC)c(OC)c(OC)c1
Mol. weight [g/mol]:	208.25
CAS:	487-11-6

Physical Properties

Property code	Value	Unit	Source
gf	-93.48	kJ/mol	Joback Method
hf	-360.12	kJ/mol	Joback Method
hfus	21.99	kJ/mol	Joback Method
hvap	53.13	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.441		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	1524.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1560.00		NIST Webbook

rinpol	1525.00	NIST Webbook
rinpol	1525.00	NIST Webbook
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ripol	2232.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2202.00		NIST Webbook
ripol	2242.00		NIST Webbook
tb	579.52	K	Joback Method
tc	780.79	K	Joback Method
tf	353.91	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.13	J/mol×K	579.52	Joback Method

cpg	470.12	J/mol×K	747.24	Joback Method
cpg	458.19	J/mol×K	713.70	Joback Method
cpg	445.60	J/mol×K	680.15	Joback Method
cpg	432.39	J/mol×K	646.61	Joback Method
cpg	418.56	J/mol×K	613.06	Joback Method
cpg	481.39	J/mol×K	780.79	Joback Method
dvisc	0.0001098	Pa×s	579.52	Joback Method
dvisc	0.0001333	Pa×s	541.92	Joback Method
dvisc	0.0001666	Pa×s	504.32	Joback Method
dvisc	0.0002159	Pa×s	466.72	Joback Method
dvisc	0.0002927	Pa×s	429.11	Joback Method
dvisc	0.0004207	Pa×s	391.51	Joback Method
dvisc	0.0006532	Pa×s	353.91	Joback Method

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=C487116&Units=SI
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical 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