Isoelemicin

Other names:	Benzene, 5(1-propenyl)-1,2,3-trimethoxy
	Isoelemicine
Inchi:	InChI=1S/C12H16O3/c1-5-6-9-7-10(13-2)12(15-4)11(8-9)14-3/h5-8H,1-4H3/b6-5+
InchiKey:	RRXOQHQFJOQLQR-AATRIKPKSA-N
Formula:	C12H16O3
SMILES:	CC=Cc1cc(OC)c(OC)c(OC)c1
Mol. weight [g/mol]:	208.25
CAS:	487-12-7

Physical Properties

Property code	Value	Unit	Source
gf	-101.10	kJ/mol	Joback Method
hf	-368.33	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.745		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1577.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1595.00		NIST Webbook
ripol	2403.00		NIST Webbook
ripol	2390.00		NIST Webbook

ripol	2399.00		NIST Webbook
tb	587.00	K	Joback Method
tc	792.75	K	Joback Method
tf	350.59	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.78	J/mol×K	587.00	Joback Method
cpg	419.37	J/mol×K	621.29	Joback Method
cpg	433.31	J/mol×K	655.58	Joback Method
cpg	446.60	J/mol×K	689.87	Joback Method
cpg	459.22	J/mol×K	724.16	Joback Method
cpg	471.18	J/mol×K	758.45	Joback Method
cpg	482.46	J/mol×K	792.75	Joback Method
dvisc	0.0006142	Pa×s	350.59	Joback Method
dvisc	0.0003804	Pa×s	389.99	Joback Method
dvisc	0.0002572	Pa×s	429.39	Joback Method
dvisc	0.0001858	Pa×s	468.80	Joback Method
dvisc	0.0001411	Pa×s	508.20	Joback Method
dvisc	0.0001115	Pa×s	547.60	Joback Method
dvisc	0.0000910	Pa×s	587.00	Joback Method

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=C487127&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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