Isoelemicin

Other names:	trans-Isoelemicin
	(E)-Isoelemicin
	(E)-isoelemicine
	trans-Isoelemicine
	(E)-1,2,3-Trimethoxy-5-(prop-1-en-1-yl)benzene
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:	5273-85-8

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	1654.20		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: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5273858&Units=SI

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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