«beta»-Asarone

Other names:	Benzene, 1,2,4-trimethoxy-5-(1-propenyl)-, (Z)-
	cis-Asarone
	cis-«beta»-Asarone
	(Z)-Asarone
	Benzene, 1,2,4-trimethoxy-5-propenyl-, (Z)-
	cis-Isoasarone
	cis-Isoelemicin
	(Z)-5-Propenyl-1,2,4-trimethoxybenzene
	(Z)-«beta»-Asarone
	(Z)-Isoelemicin
	1,2,4-Trimethoxy-5-[(1Z)-1-propenyl]benzene
	(Z)-Azarone
	2,4,5-trimethoxypropen-1-ylbenzene
Inchi:	InChI=1S/C12H16O3/c1-5-6-9-7-11(14-3)12(15-4)8-10(9)13-2/h5-8H,1-4H3/b6-5-
InchiKey:	RKFAZBXYICVSKP-WAYWQWQTSA-N
Formula:	C12H16O3
SMILES:	CC=Cc1cc(OC)c(OC)cc1OC
Mol. weight [g/mol]:	208.25
CAS:	5273-86-9

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	1596.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1641.10		NIST Webbook
rinpol	1631.00		NIST Webbook

rinpol	1583.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1579.00		NIST Webbook
ripol	2215.00		NIST Webbook
ripol	2252.00		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	471.18	J/mol×K	758.45	Joback Method
cpg	459.22	J/mol×K	724.16	Joback Method
cpg	446.60	J/mol×K	689.87	Joback Method
cpg	433.31	J/mol×K	655.58	Joback Method
cpg	419.37	J/mol×K	621.29	Joback Method
cpg	482.46	J/mol×K	792.75	Joback Method
dvisc	0.0000910	Pa×s	587.00	Joback Method
dvisc	0.0001115	Pa×s	547.60	Joback Method
dvisc	0.0001411	Pa×s	508.20	Joback Method
dvisc	0.0001858	Pa×s	468.80	Joback Method
dvisc	0.0002572	Pa×s	429.39	Joback Method
dvisc	0.0003804	Pa×s	389.99	Joback Method
dvisc	0.0006142	Pa×s	350.59	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=C5273869&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume