1,3-Cyclohexadiene, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, [S-(R*,S*)]-

Other names: (-)-Zingiberene
(3R)-3-((1S)-1,5-dimethyl-4-hexen-1-yl)-6-methylenecyclohexene
.beta.-sesquiphellandrene
Zingiberene
[S-(R*,S*)]-5-(1,5-dimethylhexen-4-yl)-2-methyl-1,3-cyclohexa-1,3-diene
l-Zingiberene
«alpha»-Zingiberene
«alpha»-zingibirene

Inchi: InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6,8-10,14-15H,5,7,11H2,1-

InchiKey: KKOXKGNSUHTUBV-UHFFFAOYSA-N

Formula: C15H24

SMILES: CC(C)=CCCC(C)C1C=CC(C)=CC1

Mol. weight [g/mol]: 204.35

CAS: 495-60-3

Physical Properties

Property code	Value	Unit	Source
gf	219.39	kJ/mol	Joback Method
hf	-92.37	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	50.31	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	1495.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1471.80		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook

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ripol	1721.00		NIST Webbook
ripol	1715.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1725.00		NIST Webbook
tb	569.05	K	Joback Method
tc	774.33	K	Joback Method
tf	246.19	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.43	J/mol×K	569.05	Joback Method
cpg	514.99	J/mol×K	603.26	Joback Method
cpg	534.40	J/mol×K	637.48	Joback Method
cpg	552.71	J/mol×K	671.69	Joback Method
cpg	569.96	J/mol×K	705.90	Joback Method
cpg	586.22	J/mol×K	740.11	Joback Method
cpg	601.53	J/mol×K	774.33	Joback Method
hvapt	74.00	kJ/mol	298.15	Vapor pressure and vaporization enthalpy studies of the major components of ginger, alpha-zingiberene, beta-sesquiphellandrene and (-) ar curcumene by correlation gas chromatography

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C495603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressure and vaporization enthalpy studies of the major components of ginger, alpha-zingiberene, beta-sesquiphellandrene and (-) ar curcumene by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2019.06.011
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
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