

Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1«alpha»,2«beta»,4«beta»)]-

Other names: Cyclohexane, 2,4-diisopropenyl-1-methyl-1-vinyl-, (1S,2R,4R)- (-)-«beta»-Elemene, (-)-(-)-«beta»-Elemene, levo-«beta»-Elemene, «beta»-Elemene, «beta»-Elemene enantiomer, 2,4-Diisopropenyl-1-methyl-1-vinylcyclohexane, [1S-(1 «alpha»,2«beta»,4«beta»)]-, Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, (1S,2S,4R)-beta elemene

Inchi: InChI=1S/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,13-14H,1-2,4,8-10H2,3,5

InchiKey: OPFTUNCRGUEPRZ-QLFBSQMISA-N

Formula: C15H24

SMILES: C=CC1(C)CCC(C(=C)C)CC1C(=C)C

Mol. weight [g/mol]: 204.35

CAS: 515-13-9

Physical Properties

Property code	Value	Unit	Source
gf	325.38	kJ/mol	Joback Method
hf	32.66	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	45.79	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.747		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
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tb	542.85	K	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.78	J/mol×K	542.85	Joback Method
cpg	511.42	J/mol×K	578.06	Joback Method
cpg	532.71	J/mol×K	613.28	Joback Method
cpg	552.77	J/mol×K	648.49	Joback Method
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cpg	589.70	J/mol×K	718.92	Joback Method
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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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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