

Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)- (3R-trans)-

Other names: p-Menth-3-ene, 2-isopropenyl-1-vinyl-, (1S,2R)-(-)-«delta»-Elemene
(3R-trans)-4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)cyclohexene
3-Isopropenyl-1-isopropyl-4-methyl-4-vinyl-1-cyclohexene-, (3R-trans)-
Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)-, (3R,4R)-
3-Isopropenyl-1-isopropyl-4-methyl-4-vinyl-1-cyclohexene-, (3R,4R)-«delta»-Elemene

Inchi: InChI=1S/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,10-11,14H,1,4,8-9H2,2-3H1

InchiKey: MXDMETWAEGIFOE-UHFFFAOYSA-N

Formula: C15H24

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

Mol. weight [g/mol]: 204.35

CAS: 20307-84-0

Physical Properties

Property code	Value	Unit	Source
gf	271.69	kJ/mol	Joback Method
hf	-21.61	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	47.26	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.747		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
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tc	765.44	K	Joback Method
tf	266.65	K	Joback Method
vc	0.749	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.92	J/mol×K	554.66	Joback Method
cpg	512.28	J/mol×K	589.79	Joback Method
cpg	532.38	J/mol×K	624.92	Joback Method
cpg	551.37	J/mol×K	660.05	Joback Method
cpg	569.35	J/mol×K	695.18	Joback Method
cpg	586.44	J/mol×K	730.31	Joback Method
cpg	602.78	J/mol×K	765.44	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

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

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