

«gamma»-Elemene

Other names:

1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane),
(1R-trans)-«gamma»-Elemene

o-Menth-8-ene, 4-isopropylidene-1-vinyl, (-)-

Elema-1,3,7-triene

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

InchiKey: BQSLMQNYHVFRDT-UHFFFAOYSA-N

Formula: C15H24

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

Mol. weight [g/mol]: 204.35

CAS: 29873-99-2

Physical Properties

Property code	Value	Unit	Source
gf	290.71	kJ/mol	Joback Method
hf	3.60	kJ/mol	Joback Method
hfus	16.36	kJ/mol	Joback Method
hvap	47.56	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1415.00		NIST Webbook
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ripol	1628.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1651.00		NIST Webbook
tb	557.48	K	Joback Method
tc	771.21	K	Joback Method
tf	264.77	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.96	J/mol×K	557.48	Joback Method
cpg	512.54	J/mol×K	593.10	Joback Method
cpg	532.84	J/mol×K	628.72	Joback Method
cpg	551.99	J/mol×K	664.35	Joback Method
cpg	570.13	J/mol×K	699.97	Joback Method
cpg	587.38	J/mol×K	735.59	Joback Method
cpg	603.88	J/mol×K	771.21	Joback Method

Sources

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=C29873992&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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