

«alpha»-Phellandrene

Other names:	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)- 2-Methyl-5-isopropyl-1,3-cyclohexadiene 2-methyl-5-(1-methylethyl)-1,3-cyclohexadiene 4-Isopropyl-1-methyl-1,5-cyclohexadiene 5-Isopropyl-2-methyl-1,3-cyclohexadiene 5-Isopropyl-2-methyl-cyclohexa-1,3-diene 5-isopropyl-2-methylcyclohexa-1,3-diene («alpha»-phellandrene) 5-isopropyl-2-methylcyclohexa-1,3-diene (Â«alphaÂ»-phellandrene) L-Phellandrene Menthadiene alpha-Phellandrene p-Mentha-1,5-diene «alpha»-Fellandrene «alpha»-Phellanderene Â«alphaÂ»-Fellandrene Â«alphaÂ»-Phellanderene
Inchi:	InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4-6,8,10H,7H2,1-3H3
InchiKey:	OGLDWXZKYODSOB-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	CC1=CCC(C(C)C)C=C1
Mol. weight [g/mol]:	136.23
CAS:	99-83-2

Physical Properties

Property code	Value	Unit	Source
gf	105.62	kJ/mol	Joback Method
hf	-96.60	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	39.14	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.165		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
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tb	450.61	K	Joback Method
tc	657.58	K	Joback Method
tf	208.88	K	Joback Method
vc	0.494	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.83	J/molxK	450.61	Joback Method
cpg	288.98	J/molxK	485.11	Joback Method
cpg	305.27	J/molxK	519.60	Joback Method
cpg	320.71	J/molxK	554.10	Joback Method
cpg	335.32	J/molxK	588.59	Joback Method
cpg	349.14	J/molxK	623.09	Joback Method
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hvapt	47.70	kJ/mol	370.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.36978e+01
Coeff. B	-3.68582e+03
Coeff. C	-5.27490e+01
Temperature range (K), min.	327.60
Temperature range (K), max.	492.25

Sources

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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
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
pvap:	Vapor 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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