

Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-

Other names:	3-Thujene «alpha»-Thujene Thujene, «alpha»- Origanene 2-Methyl-5-(1-methylethyl)-bicyclo(3.1.0)hex-2-ene 5-Isopropyl-2-methylbicyclo[3.1.0]hex-2-ene Thujene thujiene «alpha»-thuiene
Inchi:	InChI=1S/C10H16/c1-7(2)10-5-4-8(3)9(10)6-10/h4,7,9H,5-6H2,1-3H3
InchiKey:	KQAZVFVOEIRWHN-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	CC1=CCC2(C(C)C)CC12
Mol. weight [g/mol]:	136.23
CAS:	2867-05-2

Physical Properties

Property code	Value	Unit	Source
gf	167.22	kJ/mol	Joback Method
hf	-47.86	kJ/mol	Joback Method
hfus	8.94	kJ/mol	Joback Method
hvap	44.80	kJ/mol	NIST Webbook
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
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tb	445.62	K	Joback Method
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tf	260.52	K	Joback Method
vc	0.487	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.80	J/mol×K	445.62	Joback Method
cpg	292.04	J/mol×K	479.99	Joback Method
cpg	307.91	J/mol×K	514.35	Joback Method
cpg	322.57	J/mol×K	548.72	Joback Method
cpg	336.15	J/mol×K	583.09	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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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