Bicyclo[3.1.0]hex-2-ene, 4-methyl-1-(1-methylethyl)-

Other names:	2-Thujene
	«beta»-Thujene
	1-Isopropyl-4-methylbicyclo[3.1.0]hex-2-ene
Inchi:	InChI=1S/C10H16/c1-7(2)10-5-4-8(3)9(10)6-10/h4-5,7-9H,6H2,1-3H3
InchiKey:	GJYKUZUTZNTBEC-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	CC1C=CC2(C(C)C)CC12
Mol. weight [g/mol]:	136.23
CAS:	28634-89-1

Physical Properties

Property code	Value	Unit	Source
gf	169.14	kJ/mol	Joback Method
hf	-56.73	kJ/mol	Joback Method
hfus	10.40	kJ/mol	Joback Method
hvap	36.12	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.855		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	966.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	968.00		NIST Webbook
ripol	1117.00		NIST Webbook
ripol	1133.00		NIST Webbook
ripol	1107.00		NIST Webbook
tb	435.97	K	Joback Method
tc	640.39	K	Joback Method
tf	243.76	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.23	J/mol×K	435.97	Joback Method
cpg	291.43	J/mol×K	470.04	Joback Method
cpg	308.21	J/mol×K	504.11	Joback Method
cpg	323.71	J/mol×K	538.18	Joback Method
cpg	338.07	J/mol×K	572.25	Joback Method
cpg	351.42	J/mol×K	606.32	Joback Method
cpg	363.91	J/mol×K	640.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C28634891&Units=SI

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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