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

Other names: 1-Isopropyl-4-methylenebicyclo[3.1.0]hex-2-ene
2,4(10)-Thujadiene
4-Methylene-1-(1-methylethyl)-bicyclo[3.1.0]hex-2-ene
Dehydrosabinene
Thuja-2,4(10)-diene
2,4-Thujadiene
Dehydrosabinene (Thuja-2,4(10)-diene)

Inchi: InChI=1S/C10H14/c1-7(2)10-5-4-8(3)9(10)6-10/h4-5,7,9H,3,6H2,1-2H3

InchiKey: LBVRQJWOZIMWNY-UHFFFAOYSA-N

Formula: C10H14

SMILES: C=C1C=CC2(C(C)C)CC12

Mol. weight [g/mol]: 134.22

CAS: 36262-09-6

Physical Properties

Property code	Value	Unit	Source
gf	229.93	kJ/mol	Joback Method
hf	47.85	kJ/mol	Joback Method
hfus	8.17	kJ/mol	Joback Method
hvap	36.59	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.775		Crippen Method
mcvol	121.440	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	954.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	955.80		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	957.00		NIST Webbook

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rinpol	955.80		NIST Webbook
rinpol	939.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1117.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1117.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1116.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1137.00		NIST Webbook
tb	439.80	K	Joback Method
tc	646.50	K	Joback Method
tf	261.68	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	258.75	J/mol×K	439.80	Joback Method
cpg	274.99	J/mol×K	474.25	Joback Method
cpg	289.88	J/mol×K	508.70	Joback Method
cpg	303.56	J/mol×K	543.15	Joback Method
cpg	316.18	J/mol×K	577.60	Joback Method
cpg	327.87	J/mol×K	612.05	Joback Method
cpg	338.79	J/mol×K	646.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36262096&Units=SI
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

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