(-)-«alpha»-thujene

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: 3917-48-4

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
ripol	1010.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3917484&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume