(-)-(5R,6S,7S)-Aromadendra-1(10),3-diene

Inchi: InChI=1S/C15H22/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h5,12-14H,6-8H2,1-4H
InchiKey: ABTDAARSCHTOMI-IHRRRGAJSA-N
Formula: C15H22
SMILES: CC1=CCC2=C(C)CCC3C(C12)C3(C)C
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	251.30	kJ/mol	Joback Method
hf	-70.80	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	50.18	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.335		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1512.00		NIST Webbook
tb	580.19	K	Joback Method
tc	801.07	K	Joback Method
tf	364.33	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.41	J/mol×K	580.19	Joback Method
cpg	506.16	J/mol×K	617.00	Joback Method
cpg	525.61	J/mol×K	653.82	Joback Method
cpg	543.92	J/mol×K	690.63	Joback Method
cpg	561.29	J/mol×K	727.44	Joback Method
cpg	577.90	J/mol×K	764.26	Joback Method
cpg	593.92	J/mol×K	801.07	Joback Method

Sources

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=R561630&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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