(+)-(1R,5S,6S,7S)-allo-aromadendra-4(15),10(14)-d

Inchi: InChI=1S/C15H22/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h11-14H,1-2,5-8H2,3-4
InchiKey: JNXBLAGJPYZBMG-AAVRWANBSA-N
Formula: C15H22
SMILES: C=C1CCC2C(C3C(=C)CCC13)C2(C)C
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	318.72	kJ/mol	Joback Method
hf	-3.81	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	47.62	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.191		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1457.00		NIST Webbook
tb	560.58	K	Joback Method
tc	777.89	K	Joback Method
tf	348.37	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.79	J/mol×K	560.58	Joback Method
cpg	504.87	J/mol×K	596.80	Joback Method
cpg	525.53	J/mol×K	633.02	Joback Method
cpg	544.93	J/mol×K	669.23	Joback Method
cpg	563.24	J/mol×K	705.45	Joback Method
cpg	580.63	J/mol×K	741.67	Joback Method
cpg	597.27	J/mol×K	777.89	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=R406390&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

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