

(+)-aromadendra-4(15),10(14)-dien-1-ol

Inchi:	InChI=1S/C15H22O/c1-9-7-8-15(16)10(2)5-6-11-13(12(9)15)14(11,3)4/h11-13,16H,1-2,5
InchiKey:	HSEADIKPAODSBI-BHPKHCPMSA-N
Formula:	C15H22O
SMILES:	<chem>C=C1CCC2(O)C(=C)CCC3C(C12)C3(C)C</chem>
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
gf	176.41	kJ/mol	Joback Method
hf	-140.80	kJ/mol	Joback Method
hfus	16.13	kJ/mol	Joback Method
hvap	63.14	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.306		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinsol	1579.00		NIST Webbook
tb	653.00	K	Joback Method
tc	862.31	K	Joback Method
tf	433.09	K	Joback Method
vc	0.712	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.13	J/mol×K	653.00	Joback Method
cpg	567.75	J/mol×K	687.88	Joback Method
cpg	584.62	J/mol×K	722.77	Joback Method
cpg	600.96	J/mol×K	757.65	Joback Method
cpg	617.01	J/mol×K	792.54	Joback Method
cpg	632.98	J/mol×K	827.42	Joback Method
cpg	649.12	J/mol×K	862.31	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=R406414&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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