

Bicyclo[9.3.1]pentadeca-3,7-dien-12-ol, 4,8,12,15,15-pentamethyl-, [1R-(1R*,3E,7E,11R*,12R*)]-

Other names: Verticillol
Verticillol

4,8,12,15,15-Pentamethylbicyclo[9.3.1]pentadeca-3,7-dien-12-ol I-,
(1R,3E,7E,11R,12R)-
Bicyclo[9.3.1]pentadeca-3,7-dien-12-ol, 4,8,12,15,15-pentamethyl-,
(1R,3E,7E,11R,12R)-

Inchi: InChI=1S/C20H34O/c1-15-7-6-8-16(2)10-12-18-19(3,4)17(11-9-15)13-14-20(18,5)21/h8-15

InchiKey: CQWSCMMFUZYKBO-KUONJXJVSA-N

Formula: C20H34O

SMILES: CC1=CCC2CCC(C)(O)C(CCC(C)=CCC1)C2(C)C

Mol. weight [g/mol]: 290.48

CAS: 70000-19-0

Physical Properties

Property code	Value	Unit	Source
gf	7.56	kJ/mol	Joback Method
hf	-435.78	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	77.16	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.647		Crippen Method
mcvol	268.210	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2036.70		NIST Webbook
rinpol	2036.70		NIST Webbook
tb	800.51	K	Joback Method
tc	1025.42	K	Joback Method
tf	446.06	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	878.56	J/mol×K	800.51	Joback Method
cpg	903.21	J/mol×K	837.99	Joback Method
cpg	927.18	J/mol×K	875.48	Joback Method
cpg	950.68	J/mol×K	912.96	Joback Method
cpg	973.92	J/mol×K	950.45	Joback Method
cpg	997.11	J/mol×K	987.93	Joback Method
cpg	1020.46	J/mol×K	1025.42	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=C70000190&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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