

Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4Z,9S*)]-

Other names:

(-)-isocaryophyllene
(1R,9S,Z)-4,11,11-trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene
(Z)-caryophyllene
(Z)-«beta»-Caryophyllene
Bicyclo(7.2.0)undec-4-ene, 4,11,11-trimethyl-8-methylene-, (1R,4Z,9S)-
[1R-(1R*,4Z,9S*)]-4,11,11-trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene
cis-caryophyllene
isocaryophyllene
«beta»-cis-Caryophyllene
«gamma»-Caryophyllene

Inchi: InChI=1S/C15H24/c1-11-6-5-7-12(2)13-10-15(3,4)14(13)9-8-11/h6,13-14H,2,5,7-10H2,1,
InchiKey: NPNUFJAVOONJE-BJLYVFBQSA-N
Formula: C15H24
SMILES: C=C1CCC=C(C)CCC2C1CC2(C)C
Mol. weight [g/mol]: 204.35
CAS: 118-65-0

Physical Properties

Property code	Value	Unit	Source
gf	196.63	kJ/mol	Joback Method
hf	-112.68	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1411.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1402.00		NIST Webbook
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ripol	1570.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1648.00		NIST Webbook
tb	576.30	K	Joback Method
tc	802.06	K	Joback Method
tf	323.71	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.51	J/mol×K	764.43	Joback Method
cpg	501.77	J/mol×K	576.30	Joback Method
cpg	525.28	J/mol×K	613.93	Joback Method
cpg	547.37	J/mol×K	651.55	Joback Method
cpg	568.18	J/mol×K	689.18	Joback Method
cpg	587.84	J/mol×K	726.81	Joback Method
cpg	624.31	J/mol×K	802.06	Joback Method
hvapt	66.00	kJ/mol	298.15	Thermochemical properties of sesquiterpenes in natural products by correlation gas chromatography: Application to bergamotene oil

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical properties of sesquiterpenes in natural products by Joback Method:	https://www.doi.org/10.1016/j.jct.2018.06.017
Application to bergamotene oil: McGowan Method:	https://en.wikipedia.org/wiki/Joback_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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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