

Caryophyllene

Other names:

(-)-(E)-Caryophyllene
(-)-.beta.-caryophyllene
(-)-E-caryophyllene
(-)-caryophyllene
(-)-trans-caryophyllene
(E)-Caryophyllene
(E)-«beta»-Caryophyllene
.beta.-caryophyllen
.beta.-caryophyllene
.beta.-caryophyllene, (-)
4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene
8-Methylene-4,11,11-(trimethyl)bicyclo(7.2.0)undec-4-ene, (1R,4E,9S)-
Bicyclo(7.2.0)undec-4-ene, 8-methylene-4,11,11-trimethyl-, (E)-(1R,9S)-(-)-
Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (E)-(1R,9S)-(-)-
Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]-
Caryophyllene B
Caryophyllene, (E)
E-«beta»-Caryophyllene
NSC 11906
[1R-(1R*,4E,9S*)]-4,11,11-trimethyl-8-methylene-bicyclo[7.2.0]-4-undecene
[1R-(1R*,4E,9S*)]-8-methylene-4,11,11-trimethylbicyclo[7.2.0]-4-undecene
beta-Caryophyllene
bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (E)-(1R,9S)-(-)-
bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]-
bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-[1R-(4E,9S)]
l-caryophyllene
t-«beta»-Caryophyllene
trans-caryophyllene
trans-«beta»-Caryophyllene
«beta»-(E)-Caryophyllene
«beta»-Caryophyllene
«beta»-Caryophyllen
«beta»-Caryophyllene
«beta»-cariofillene
«beta»-caryophellene
«beta»-trans-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-IOMPXFEGSA-N

Formula:

C15H24

SMILES:

C=C1CCC=C(C)CCC2C1CC2(C)C

Mol. weight [g/mol]: 204.35
CAS: 87-44-5

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	65.50	kJ/mol	NIST Webbook
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1419.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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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	606.51	J/mol×K	764.43	Joback Method
cpg	624.31	J/mol×K	802.06	Joback Method
pvap	101.33	kPa	526.40	Measurement and correlation of vapor-liquid equilibrium data for binary systems composed of camphene, (+)-3-carene, (-)-beta-caryophyllene, p-cymene, and alpha-pinene at 101.33 kPa
pvap	101.33	kPa	526.53	Measurement and correlation of vapor-liquid equilibrium data for binary systems composed of camphene, (+)-3-carene, (-)-beta-caryophyllene, p-cymene, and alpha-pinene at 101.33 kPa
pvap	101.33	kPa	526.47	Measurement and correlation of vapor-liquid equilibrium data for binary systems composed of camphene, (+)-3-carene, (-)-beta-caryophyllene, p-cymene, and alpha-pinene at 101.33 kPa

rhoI	896.80	kg/m3	298.15	Measurement and correlation of vapor-liquid equilibrium data for binary and ternary systems composed of (-)-beta-caryophyllene, p-cymene and 3-carene at 101.33 kPa
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

High-pressure phase equilibrium data for systems with carbon dioxide, measurement and correlation of vapor-liquid equilibrium data for binary and ternary systems composed of (-)-beta-caryophyllene, p-cymene and 3-carene at 101.33 kPa: <https://www.doi.org/10.1016/j.jct.2008.07.006>

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Measurement and correlation of vapor-liquid equilibrium data for binary and ternary systems composed of (-)-beta-caryophyllene, p-cymene and 3-carene at 101.33 kPa: <https://www.doi.org/10.1016/j.tca.2019.178318>

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=C87445&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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
pvap:	Vapor pressure
rhoI:	Liquid Density
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

Latest version available from:

<https://www.chemeo.com/cid/70-147-1/Caryophyllene.pdf>

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