Bicyclo[3.1.1]heptane, 6-methyl-2-methylene-6-(4-methyl-3-pentenyl)-, [1R-(1«alpha»,5«alpha»,6«beta»)]-

Other names: (-)-.beta.-caryophyllene
(-)-E-caryophyllene
(-)-caryophyllene
(-)-trans-caryophyllene
(E)-«beta»-Bergamotene
.beta.-caryophyllen
.beta.-caryophyllene
.beta.-caryophyllene, (-)
6-Methyl-2-methylene-6-(4-methyl-3-pentenyl)-bicyclo[3.1.1]heptane
6-Methyl-2-methylene-6-(4-methyl-3-pentenyl)bicyclo[3.1.1]heptane-, [1R-(1«alpha»,5«alpha»,6«beta»)]-
Bergamotene
[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
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
l-caryophyllene
trans-caryophyllene
trans-«beta»-bergamotene

Inchi: InChI=1S/C15H24/c1-11(2)6-5-9-15(4)13-8-7-12(3)14(15)10-13/h6,13-14H,3,5,7-10H2,1-

InchiKey: DGZBGCMPRYFWFF-UHFFFAOYSA-N

Formula: C15H24

SMILES: C=C1CCC2CC1C2(C)CCC=C(C)C

Mol. weight [g/mol]: 204.35

CAS: 55123-21-2

Physical Properties

Property code	Value	Unit	Source
gf	296.37	kJ/mol	Joback Method
hf	-26.92	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1486.00		NIST Webbook

rinpol	1480.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1475.00	NIST Webbook
rinpol	1479.00	NIST Webbook
rinpol	1427.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1467.00	NIST Webbook
rinpol	1436.00	NIST Webbook
rinpol	1430.00	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1484.00	NIST Webbook
rinpol	1471.00	NIST Webbook
rinpol	1480.00	NIST Webbook
rinpol	1470.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1436.00	NIST Webbook
rinpol	1479.00	NIST Webbook
rinpol	1479.00	NIST Webbook
rinpol	1479.00	NIST Webbook
rinpol	1433.00	NIST Webbook
rinpol	1475.00	NIST Webbook
rinpol	1476.00	NIST Webbook
rinpol	1486.00	NIST Webbook
rinpol	1475.00	NIST Webbook
rinpol	1485.00	NIST Webbook
rinpol	1427.00	NIST Webbook
ripol	1586.00	NIST Webbook
ripol	1594.00	NIST Webbook
ripol	1594.00	NIST Webbook
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ripol	1594.00	NIST Webbook
ripol	1595.00	NIST Webbook
ripol	1594.00	NIST Webbook
ripol	1594.00	NIST Webbook
ripol	1594.00	NIST Webbook
ripol	1586.00	NIST Webbook

ripol	1588.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1594.00		NIST Webbook
tb	559.12	K	Joback Method
tc	765.28	K	Joback Method
tf	305.47	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.48	J/mol×K	559.12	Joback Method
cpg	516.19	J/mol×K	593.48	Joback Method
cpg	535.61	J/mol×K	627.84	Joback Method
cpg	553.91	J/mol×K	662.20	Joback Method
cpg	571.23	J/mol×K	696.56	Joback Method
cpg	587.73	J/mol×K	730.92	Joback Method
cpg	603.56	J/mol×K	765.28	Joback Method
hvapt	65.90	kJ/mol	298.15	Thermochemical properties of sesquiterpenes in natural products by correlation gas chromatography: Application to bergamotene oil

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical properties of sesquiterpenes in natural products by correlation gas chromatography: Application to bergamotene oil:	https://www.doi.org/10.1016/j.jct.2018.06.017
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=C55123212&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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