

Caryophyllene oxide

Other names:

5-Oxatricyclo[8.2.0.0(4,6)]dodecane, 4,12,12-trimethyl-9-methylene-,
[1R-(1R*,4R*,6R*,10S*)]-
5-Oxatricyclo[8.2.0.0(4,6)]dodecane, 4,12,12-trimethyl-9-methylene-,
(1R,4R,6R,10S)-
Caryophyllene oxide

Caryophyllene epoxide

(-)-«beta»-Caryophyllene epoxide

«beta»-Caryophyllene oxide

Epoxyaryophyllene

(-)-Epoxydihydroaryophyllene

4,11,11-Trimethyl-8-methylene-5-oxatricyclo(8.2.0.0(4,6))dodecane,

(1R,4R,6R,10S)-

(-)-5-Oxatricyclo[8.2.0.0(4,6)]dodecane,4,12,12-trimethyl-9-methylene-,

[1R-(1R*,4R*,6R*,10S*)]-

«beta»-Caryophyllene epoxide

(-)-«beta»-Caryophyllene oxide

Caryophyllene oxyde

4,12,12-trimethyl-9-methylene-5-oxatricyclo[8.2.0.]dodecane (caryophyllene oxide)

[1R-(1R*,4R*,6R*,10S*)]-4,12,12-trimethyl-9-methylene-5-oxatricyclo[8.2.0.04,6]dodecane

Inchi:

InChI=1S/C15H24O/c1-10-5-6-13-15(4,16-13)8-7-12-11(10)9-14(12,2)3/h11-13H,1,5-9H2

InchiKey:

NVEQFIOZRFFVFW-COMQUAJESA-N

Formula:

C15H24O

SMILES:

C=C1CCC2OC2(C)CCC2C1CC2(C)C

Mol. weight [g/mol]:

220.35

CAS:

1139-30-6

Physical Properties

Property code	Value	Unit	Source
gf	161.93	kJ/mol	Joback Method
hf	-210.97	kJ/mol	Joback Method
hfus	19.08	kJ/mol	Joback Method
hvap	50.99	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.936		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
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ripol	2032.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	2014.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	2014.00		NIST Webbook
tb	592.88	K	Joback Method
tc	822.50	K	Joback Method
tf	381.64	K	Joback Method
vc	0.722	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.37	J/mol×K	592.88	Joback Method
cpg	562.46	J/mol×K	631.15	Joback Method
cpg	584.07	J/mol×K	669.42	Joback Method
cpg	604.52	J/mol×K	707.69	Joback Method
cpg	624.09	J/mol×K	745.96	Joback Method
cpg	643.08	J/mol×K	784.23	Joback Method
cpg	661.78	J/mol×K	822.50	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1139306&Units=SI

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
ripol:	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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