Caryophyllenol II

Other names: caryophylla-2(12),6-dien-5«beta»-ol (caryophyllenol II)
[1R-(1R*,3E,5R*,9S*)]-4,11,11-trimethyl-8-methylenebicyclo[7.2.0]undec-3-en-5-ol
Inchi: InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h5,12-14,16H,1,6-9
InchiKey: DWUYGFWOANEJRE-WZUFQYTHSA-N
Formula: C15H24O
SMILES: C=C1CCC(O)C(C)=CCC2C1CC2(C)C
Mol. weight [g/mol]: 220.35
CAS: 32214-89-4

Physical Properties

Property code	Value	Unit	Source
gf	52.10	kJ/mol	Joback Method
hf	-285.25	kJ/mol	Joback Method
hfus	19.98	kJ/mol	Joback Method
hvap	65.69	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	1633.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1655.00		NIST Webbook
ripol	2392.00		NIST Webbook
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ripol	2396.00		NIST Webbook
ripol	2396.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2350.00		NIST Webbook
tb	663.81	K	Joback Method
tc	872.81	K	Joback Method
tf	380.29	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.12	J/mol×K	663.81	Joback Method
cpg	595.62	J/mol×K	698.64	Joback Method
cpg	614.14	J/mol×K	733.48	Joback Method
cpg	631.79	J/mol×K	768.31	Joback Method
cpg	648.66	J/mol×K	803.14	Joback Method
cpg	664.87	J/mol×K	837.98	Joback Method
cpg	680.52	J/mol×K	872.81	Joback Method

Sources

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=C32214894&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
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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