

Caryophylla-2(12),6-dien-5-«alpha»-ol

Other names:	caryophylla-2(12),6-dien-5«alpha»-ol (= caryophyllenol I)
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-RJRMUTBASA-N
Formula:	C15H24O
SMILES:	C=C1CCC(O)C(C)=CCC2C1CC2(C)C
Mol. weight [g/mol]:	220.35

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
ripol	2353.00		NIST Webbook
ripol	2389.00		NIST Webbook
ripol	2389.00		NIST Webbook
ripol	2389.00		NIST Webbook
ripol	2389.00		NIST Webbook
ripol	2389.00		NIST Webbook
ripol	2364.00		NIST Webbook
ripol	2389.00		NIST Webbook
ripol	2389.00		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
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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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R236790&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:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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