

Exo methylene isomer of Caryophyllenol I

Other names:	«beta»-Caryophylla-4(14),8(15)-dien-5-ol
Inchi:	InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h12-14,16H,1-2,5-9
InchiKey:	CIYOYPOMGIECX-IHRRRGAJSA-N
Formula:	C15H24O
SMILES:	<chem>C=C1CCC2C(CC2(C)C)C(=C)CCC1O</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	84.85	kJ/mol	Joback Method
hf	-247.32	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	64.90	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1639.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1639.00		NIST Webbook
tb	658.83	K	Joback Method
tc	866.81	K	Joback Method
tf	380.69	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.21	J/molxK	658.83	Joback Method
cpg	594.89	J/molxK	693.49	Joback Method
cpg	613.57	J/molxK	728.16	Joback Method
cpg	631.35	J/molxK	762.82	Joback Method
cpg	648.34	J/molxK	797.48	Joback Method

cpg	664.64	J/mol×K	832.14	Joback Method
cpg	680.34	J/mol×K	866.81	Joback Method

Sources

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=R330713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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