

Caryophylla-2(12),6-dien-5 «beta»-ol (=Caryophylladienol II)

Inchi:	InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h5,13-14,16H,6-9H2
InchiKey:	AHWWWENJXIHBBP-HFNNDJBXSA-N
Formula:	C15H24O
SMILES:	CC1=CCC2C(=C(C)CCC1O)CC2(C)C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	17.43	kJ/mol	Joback Method
hf	-314.31	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	67.46	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.840		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
ripol	2392.00		NIST Webbook
tb	678.44	K	Joback Method
tc	889.36	K	Joback Method
tf	396.65	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.76	J/molxK	678.44	Joback Method
cpg	593.47	J/molxK	713.59	Joback Method
cpg	611.28	J/molxK	748.75	Joback Method
cpg	628.31	J/molxK	783.90	Joback Method
cpg	644.67	J/molxK	819.05	Joback Method
cpg	660.47	J/molxK	854.20	Joback Method
cpg	675.83	J/molxK	889.36	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=R438129&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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