

14-Hydroxy-9-epi-(E)-caryophyllene

Inchi:	InChI=1S/C15H24O/c1-11-5-4-6-12(10-16)7-8-14-13(11)9-15(14,2)3/h6,13-14,16H,1,4-5
InchiKey:	MGIQTXDHQJGPEZ-PJWHXWNJSA-N
Formula:	C15H24O
SMILES:	<chem>C=C1CCC=C(CO)CCC2C1CC2(C)C</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
hfus	18.91	kJ/mol	Joback Method
hvap	93.90	kJ/mol	Cheméo Relay (1.0)
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
tb	586.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.23	J/mol×K	668.48	Joback Method
cpg	593.26	J/mol×K	703.32	Joback Method
cpg	611.33	J/mol×K	738.17	Joback Method
cpg	628.56	J/mol×K	773.01	Joback Method
cpg	645.05	J/mol×K	807.85	Joback Method
cpg	660.93	J/mol×K	842.69	Joback Method
cpg	676.30	J/mol×K	877.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R607197&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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