14-Hydroxy-9-epi-«beta»-caryophyllene

Other names: 14-Hydroxy-9-epi-«beta»-Caryophyllen
Inchi: InChI=1S/C15H24O/c1-11-5-4-6-12(2)13-9-15(3,10-16)14(13)8-7-11/h5,13-14,16H,2,4,6-
InchiKey: DFMBJBXEHZSTJQ-VMLHABITSA-N
Formula: C15H24O
SMILES: C=C1CCC=C(C)CCC2C1CC2(C)CO
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	59.81	kJ/mol	Joback Method
hf	-264.91	kJ/mol	Joback Method
hfus	18.91	kJ/mol	Joback Method
hvap	66.00	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	1664.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1664.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2310.00		NIST Webbook
tb	668.48	K	Joback Method
tc	877.54	K	Joback Method
tf	384.53	K	Joback Method
vc	0.736	m3/kmol	Joback Method

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

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=R206289&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
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