4,5-Dihydro-«beta»-caryophyllene-14-al

Inchi: InChI=1S/C15H24O/c1-11-5-4-6-12(10-16)7-8-14-13(11)9-15(14,2)3/h10,12-14H,1,4-9H2
InchiKey: QRSRVOUYGXKOHE-UHFFFAOYSA-N
Formula: C15H24O
SMILES: C=C1CCCC(C=O)CCC2C1CC2(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	69.07	kJ/mol	Joback Method
hf	-264.91	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	54.78	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.984		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
ripol	2092.00		NIST Webbook
ripol	2092.00		NIST Webbook
tb	616.15	K	Joback Method
tc	840.92	K	Joback Method
tf	348.19	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.16	J/mol×K	616.15	Joback Method
cpg	575.19	J/mol×K	653.61	Joback Method
cpg	596.86	J/mol×K	691.07	Joback Method
cpg	617.30	J/mol×K	728.54	Joback Method
cpg	636.65	J/mol×K	766.00	Joback Method
cpg	655.04	J/mol×K	803.46	Joback Method
cpg	672.59	J/mol×K	840.92	Joback Method

Sources

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=R336197&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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