caryophylla-2(12),6-dien-5-one

Inchi: InChI=1S/C15H22O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h5,12-13H,1,6-9H2,
InchiKey: UVPVOJNEDSOAHT-CGGDQNISSA-N
Formula: C15H22O
SMILES: C=C1CCC(=O)C(C)=CCC2C1CC2(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	74.04	kJ/mol	Joback Method
hf	-250.38	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	53.57	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
ripol	2079.00		NIST Webbook
tb	644.12	K	Joback Method
tc	882.69	K	Joback Method
tf	391.93	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.17	J/mol×K	644.12	Joback Method
cpg	564.63	J/mol×K	683.88	Joback Method
cpg	585.82	J/mol×K	723.64	Joback Method
cpg	605.89	J/mol×K	763.41	Joback Method
cpg	624.93	J/mol×K	803.17	Joback Method
cpg	643.09	J/mol×K	842.93	Joback Method
cpg	660.47	J/mol×K	882.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R330926&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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