caryophylla-4(12),8(13)-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/h12-13H,1-2,5-9H2,
InchiKey: ZZHHIRFCRIFTAN-STQMWFEESA-N
Formula: C15H22O
SMILES: C=C1CCC2C(CC2(C)C)C(=C)CCC1=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	106.79	kJ/mol	Joback Method
hf	-212.45	kJ/mol	Joback Method
hfus	12.34	kJ/mol	Joback Method
hvap	52.78	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
ripol	2028.00		NIST Webbook
ripol	2028.00		NIST Webbook
tb	639.14	K	Joback Method
tc	876.58	K	Joback Method
tf	392.33	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.15	J/mol×K	639.14	Joback Method
cpg	563.82	J/mol×K	678.71	Joback Method
cpg	585.20	J/mol×K	718.29	Joback Method
cpg	605.43	J/mol×K	757.86	Joback Method
cpg	624.62	J/mol×K	797.43	Joback Method
cpg	642.88	J/mol×K	837.00	Joback Method
cpg	660.33	J/mol×K	876.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R335134&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