

Caryophylla-2(12),6(13)-dien-5-one

Other names:	Caryophylla-2(12),6(13)-diene-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-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	<chem>C=C1CCC2C(CC2(C)C)C(=C)CCC1=O</chem>
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	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
tb	639.14	K	Joback Method
tc	876.58	K	Joback Method
tf	392.33	K	Joback Method
vc	0.722	m ³ /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

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=R237535&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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