

Caryophylla-3,8(15)-dien-5-one

Inchi:	InChI=1S/C15H24O/c1-12-7-8-14(16)13(2)6-5-10-15(3,4)11-9-12/h6H,1,5,7-11H2,2-4H3
InchiKey:	ODYWEDCMANZQIY-MLPAPPSSSA-N
Formula:	C15H24O
SMILES:	<chem>C=C1CCC(=O)C(C)=CCCC(C)(C)CC1</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	-15.30	kJ/mol	Joback Method
hf	-321.32	kJ/mol	Joback Method
hfus	8.83	kJ/mol	Joback Method
hvap	54.48	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.438		Crippen Method
mvol	204.320	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1581.00		NIST Webbook
tb	654.86	K	Joback Method
tc	900.64	K	Joback Method
tf	367.67	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.19	J/mol×K	654.86	Joback Method
cpg	586.47	J/mol×K	695.82	Joback Method
cpg	609.35	J/mol×K	736.79	Joback Method
cpg	630.89	J/mol×K	777.75	Joback Method
cpg	651.17	J/mol×K	818.71	Joback Method
cpg	670.24	J/mol×K	859.68	Joback Method
cpg	688.17	J/mol×K	900.64	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R227315&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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