«beta»-Caryophyllene, 14-oxy

Inchi: InChI=1S/C15H24O/c1-11-5-4-6-12(10-16)7-8-14-13(11)9-15(14,2)3/h6,13-14,16H,1,4-5
InchiKey: MGIQTXDHQJGPEZ-DCOFTTSXSA-N
Formula: C15H24O
SMILES: C=C1CCC=C(CO)CCC2C1CC2(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	59.81	kJ/mol	Joback Method
hf	-264.91	kJ/mol	Joback Method
hfus	18.91	kJ/mol	Joback Method
hvap	66.00	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
ripol	2357.00		NIST Webbook
tb	668.48	K	Joback Method
tc	877.54	K	Joback Method
tf	384.53	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.23	J/mol×K	668.48	Joback Method
cpg	593.26	J/mol×K	703.32	Joback Method
cpg	611.33	J/mol×K	738.17	Joback Method
cpg	628.56	J/mol×K	773.01	Joback Method
cpg	645.05	J/mol×K	807.85	Joback Method
cpg	660.93	J/mol×K	842.69	Joback Method
cpg	676.30	J/mol×K	877.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410389&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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