caryophyllene formate

Inchi: InChI=1S/C16H26O2/c1-14(2)9-13-12(14)5-8-15(3)6-4-7-16(13,10-15)18-11-17/h11-13H
InchiKey: BGEIOYHSLPDHJC-UHFFFAOYSA-N
Formula: C16H26O2
SMILES: CC12CCCC(OC=O)(C1)C1CC(C)(C)C1CC2
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	-6.62	kJ/mol	Joback Method
hf	-386.41	kJ/mol	Joback Method
hfus	12.03	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.935		Crippen Method
mcvol	211.160	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1559.00		NIST Webbook
tb	660.97	K	Joback Method
tc	894.12	K	Joback Method
tf	440.79	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.19	J/mol×K	660.97	Joback Method
cpg	657.72	J/mol×K	699.83	Joback Method
cpg	679.40	J/mol×K	738.69	Joback Method
cpg	700.63	J/mol×K	777.54	Joback Method
cpg	721.82	J/mol×K	816.40	Joback Method
cpg	743.39	J/mol×K	855.26	Joback Method
cpg	765.74	J/mol×K	894.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R239873&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume