(+)-Eudesma-3,7(11)-dien-8-one

Inchi: InChI=1S/C15H22O/c1-10(2)12-8-13-11(3)6-5-7-15(13,4)9-14(12)16/h6,13H,5,7-9H2,1-4
InchiKey: LLUFBBLIDQULSW-UHFFFAOYSA-N
Formula: C15H22O
SMILES: CC1=CCCC2(C)CC(=O)C(=C(C)C)CC12
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	77.68	kJ/mol	Joback Method
hf	-241.88	kJ/mol	Joback Method
hfus	15.53	kJ/mol	Joback Method
hvap	54.42	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1745.00		NIST Webbook
tb	651.88	K	Joback Method
tc	891.67	K	Joback Method
tf	382.41	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.30	J/mol×K	651.88	Joback Method
cpg	560.66	J/mol×K	691.85	Joback Method
cpg	580.83	J/mol×K	731.81	Joback Method
cpg	599.99	J/mol×K	771.78	Joback Method
cpg	618.29	J/mol×K	811.74	Joback Method
cpg	635.88	J/mol×K	851.71	Joback Method
cpg	652.93	J/mol×K	891.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R504375&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