Eudesma-4(15),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/h13H,3,5-9H2,1-2,4
InchiKey: NKGSEACIYQINQJ-WUJWULDRSA-N
Formula: C15H22O
SMILES: C=C1CCCC2(C)CC(=O)C(=C(C)C)CC12
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	110.43	kJ/mol	Joback Method
hf	-203.95	kJ/mol	Joback Method
hfus	13.54	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1707.00		NIST Webbook
tb	646.90	K	Joback Method
tc	885.57	K	Joback Method
tf	382.81	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.47	J/mol×K	646.90	Joback Method
cpg	560.03	J/mol×K	686.68	Joback Method
cpg	580.39	J/mol×K	726.46	Joback Method
cpg	599.70	J/mol×K	766.24	Joback Method
cpg	618.11	J/mol×K	806.02	Joback Method
cpg	635.78	J/mol×K	845.79	Joback Method
cpg	652.86	J/mol×K	885.57	Joback Method

Sources

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=R424145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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