10-epi-Acora-3,11-dien-15-al

Inchi: InChI=1S/C15H22O/c1-11(2)14-5-4-13(10-16)15(14)8-6-12(3)7-9-15/h6,10,13-14H,1,4-5
InchiKey: MGIKIGACFAHMIV-QLFBSQMISA-N
Formula: C15H22O
SMILES: C=C(C)C1CCC(C=O)C12CC=C(C)CC2
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	135.42	kJ/mol	Joback Method
hf	-160.70	kJ/mol	Joback Method
hfus	17.78	kJ/mol	Joback Method
hvap	55.12	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1725.00		NIST Webbook
rinpol	1726.00		NIST Webbook
ripol	2380.00		NIST Webbook
ripol	2380.00		NIST Webbook
tb	618.09	K	Joback Method
tc	845.12	K	Joback Method
tf	339.83	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.69	J/mol×K	618.09	Joback Method
cpg	548.77	J/mol×K	655.93	Joback Method
cpg	568.56	J/mol×K	693.77	Joback Method
cpg	587.20	J/mol×K	731.60	Joback Method
cpg	604.88	J/mol×K	769.44	Joback Method
cpg	621.77	J/mol×K	807.28	Joback Method

cpg	638.01	J/mol×K	845.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198504&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume