10-epi-Acor-3-en-5-one

Inchi: InChI=1S/C15H22O/c1-10(2)13-6-5-12(4)15(13)8-7-11(3)9-14(15)16/h9,12-13H,1,5-8H2,
InchiKey: BGHWWBSODRCFDG-YDHLFZDLSA-N
Formula: C15H22O
SMILES: C=C(C)C1CCC(C)C12CCC(C)=CC2=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	112.35	kJ/mol	Joback Method
hf	-212.82	kJ/mol	Joback Method
hfus	15.00	kJ/mol	Joback Method
hvap	52.65	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1650.00		NIST Webbook
ripol	2190.00		NIST Webbook
tb	637.25	K	Joback Method
tc	875.13	K	Joback Method
tf	366.05	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.13	J/mol×K	637.25	Joback Method
cpg	562.46	J/mol×K	676.90	Joback Method
cpg	583.51	J/mol×K	716.54	Joback Method
cpg	603.42	J/mol×K	756.19	Joback Method
cpg	622.34	J/mol×K	795.83	Joback Method
cpg	640.42	J/mol×K	835.48	Joback Method
cpg	657.81	J/mol×K	875.13	Joback Method

Sources

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=R198480&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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