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

Inchi: InChI=1S/C15H28O/c1-11(2)14-5-4-12(3)15(14)8-6-13(10-16)7-9-15/h11-14,16H,4-10H2
InchiKey: WZSRLLWMYRQPRW-FSJTYKKLSA-N
Formula: C15H28O
SMILES: CC(C)C1CCC(C)C12CCC(CO)CC2
Mol. weight [g/mol]: 224.38

Physical Properties

Property code	Value	Unit	Source
gf	-11.65	kJ/mol	Joback Method
hf	-414.92	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.857		Crippen Method
mcvol	206.360	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1730.00		NIST Webbook
ripol	2545.00		NIST Webbook
tb	655.80	K	Joback Method
tc	858.48	K	Joback Method
tf	341.85	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.49	J/mol×K	655.80	Joback Method
cpg	641.60	J/mol×K	689.58	Joback Method
cpg	661.63	J/mol×K	723.36	Joback Method
cpg	680.69	J/mol×K	757.14	Joback Method
cpg	698.90	J/mol×K	790.92	Joback Method
cpg	716.37	J/mol×K	824.70	Joback Method
cpg	733.22	J/mol×K	858.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R397756&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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