9-Hydroxyladanifer-10-one [9(10-->1)-abeo-9-Hydroxyaromadendran-10-one]

Inchi: InChI=1S/C15H24O2/c1-8-5-6-15(9(2)16)11(17)7-10-13(12(8)15)14(10,3)4/h8,10-13,17H

InchiKey: ZHGFRCFUYDAZGE-QMOOCHOPSA-N

Formula: C15H24O2

SMILES: CC(=O)C12CCC(C)C1C1C(CC2O)C1(C)C

Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-61.99	kJ/mol	Joback Method
hf	-456.38	kJ/mol	Joback Method
hfus	24.29	kJ/mol	Joback Method
hvap	68.78	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.645		Crippen Method
mcvol	197.070	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	1704.00		NIST Webbook
rinpol	1704.00		NIST Webbook
ripol	2559.00		NIST Webbook
ripol	2559.00		NIST Webbook
tb	694.94	K	Joback Method
tc	901.64	K	Joback Method
tf	450.70	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.20	J/mol×K	694.94	Joback Method
cpg	641.58	J/mol×K	729.39	Joback Method
cpg	659.36	J/mol×K	763.84	Joback Method
cpg	676.77	J/mol×K	798.29	Joback Method
cpg	694.04	J/mol×K	832.74	Joback Method
cpg	711.39	J/mol×K	867.19	Joback Method

cpg	729.05	J/mol×K	901.64	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=R228927&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