humuladienone

Inchi: InChI=1S/C15H24O/c1-12-7-8-14(16)13(2)6-5-10-15(3,4)11-9-12/h5,9-10,13H,6-8,11H2,
InchiKey: XWFINABYEHNSEP-VKLURXMVSA-N
Formula: C15H24O
SMILES: CC1=CCC(C)(C)C=CCC(C)C(=O)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	-46.13	kJ/mol	Joback Method
hf	-368.12	kJ/mol	Joback Method
hfus	12.28	kJ/mol	Joback Method
hvap	54.31	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.294		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1580.00		NIST Webbook
ripol	1952.00		NIST Webbook
ripol	1952.00		NIST Webbook
tb	650.19	K	Joback Method
tc	896.37	K	Joback Method
tf	350.51	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.67	J/mol×K	650.19	Joback Method
cpg	589.54	J/mol×K	691.22	Joback Method
cpg	612.94	J/mol×K	732.25	Joback Method
cpg	634.96	J/mol×K	773.28	Joback Method
cpg	655.65	J/mol×K	814.31	Joback Method
cpg	675.09	J/mol×K	855.34	Joback Method
cpg	693.34	J/mol×K	896.37	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=R237644&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