Salvialenone

Inchi: InChI=1S/C15H24O/c1-10(2)12-7-8-15(4)13(12)9-11(3)5-6-14(15)16/h10,12-13H,3,5-9H
InchiKey: JBOONPKUPONSIB-JHIQODARSA-N
Formula: C15H24O
SMILES: C=C1CCC(=O)C2(C)CCC(C(C)C)C2C1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	63.37	kJ/mol	Joback Method
hf	-295.81	kJ/mol	Joback Method
hfus	12.08	kJ/mol	Joback Method
hvap	52.06	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.984		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1586.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1608.00		NIST Webbook
tb	635.27	K	Joback Method
tc	867.84	K	Joback Method
tf	367.17	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.21	J/mol×K	635.27	Joback Method
cpg	585.42	J/mol×K	674.03	Joback Method
cpg	607.31	J/mol×K	712.79	Joback Method
cpg	628.03	J/mol×K	751.56	Joback Method
cpg	647.71	J/mol×K	790.32	Joback Method
cpg	666.46	J/mol×K	829.08	Joback Method
cpg	684.43	J/mol×K	867.84	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=R288216&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume