Zearalenone

Other names: 1H-2-Benzoxacyclotetradecin-1,7(8H)-dione, 3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-, [S-(E)]-
1H-2-Benzoxacyclotetradecin-1,7(8H)-dione, 3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-, (S)-(-)-
(S)-Zearalenone
trans-Zearalenone
Compound F-2
FES
Mycotoxin F 2
Toxin F2
(-)-Zearalenone
14,16-Dihydroxy-3-methyl-3,4,5,6,9,10-hexahydro-1H-2-benzoxacyclotetradecine-1,7(8H)
[S-(E)]-
(10S)-Zearalenone
(S)-(-)-Zearalenone
1H-2-Benzoxacyclotetradecin-1,7(8H)-dione, 3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-, (3S,11E)-
6-(10-Hydroxy-6-oxo-trans-1-undecenyl)-«beta»-resorcylic acid lactone
Zenone
[S-(E)]-3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-1H-2-benzoxacyclotetradecin-1

Inchi: InChI=1S/C18H22O5/c1-12-6-5-9-14(19)8-4-2-3-7-13-10-15(20)11-16(21)17(13)18(22)23

InchiKey: MBMQEIFVQACCCH-QDBLGGKGSA-N

Formula: C18H22O5

SMILES: CC1CCCC(=O)CCCC=Cc2cc(O)cc(O)c2C(=O)O1

Mol. weight [g/mol]: 318.36

CAS: 18695-28-8

Physical Properties

Property code	Value	Unit	Source
gf	-455.27	kJ/mol	Joback Method
hf	-876.67	kJ/mol	Joback Method
hfus	35.05	kJ/mol	Joback Method
hvap	99.39	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.580		Crippen Method
mcvol	246.310	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	2867.00		NIST Webbook
rinpol	2867.00		NIST Webbook
tb	1011.06	K	Joback Method
tc	1296.07	K	Joback Method

tf	705.03	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.96	J/mol×K	1011.06	Joback Method
cpg	870.56	J/mol×K	1058.56	Joback Method
cpg	881.90	J/mol×K	1106.06	Joback Method
cpg	891.02	J/mol×K	1153.57	Joback Method
cpg	897.99	J/mol×K	1201.07	Joback Method
cpg	902.83	J/mol×K	1248.57	Joback Method
cpg	905.60	J/mol×K	1296.07	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=C18695288&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