Diacetoxyscirpenol

Other names: Trichothec-9-ene-3,4,15-triol, 12,13-epoxy-, 4,15-diacetate, (3«alpha»,4«beta»)-
Anguidin
Anguidine
ANG 66
MM 4462
Spiro(2,5-methano-1-benzoxepin-10,2'-oxirane)-5a(6H)-methanol, 2,3,4,5,7,9a-hexahydro-3,4-dihydroxy-5,8-dimethyl-, 4,5a-diacetate
Trichothec-9-ene-3«alpha»,4«beta»,15-triol, 12,13-epoxy-, 4,15-diacetate
Trichothec-9-ene-3,4,15-triol, 12,13-epoxy-, 4,15-diacetate
Trichothec-9-ene, 12,13-epoxy-4«beta»,15-diazetoxy-3«alpha»-hydroxy-
4«beta»,15-Diacetoxy-3«alpha»-hydroxy-12,13-epoxytrichothec-9-ene
4,15-Diacetoxyscirpen-3-ol
DAS
Diazetoxyskirpenol
NSC-141537
Trichothec-9-ene, 12,13-epoxy-4-«beta»,15-diacetoxy-3-«alpha»-hydroxy-
4,15-Diacetoxyscirp-9-en-3-ol
4,15-Diacetoxyscirpenol
4,15-Di-O-acetylscirpenol
Scirp-9-ene-3«alpha»,4«beta»,15-triol, 4,15-diacetate
Scirpenetriol 4,15-diacetate
12,13-epoxytrichothec-9-ene-3«alpha»,4«beta»,15-triol 4,15-diacetate

Inchi: InChI=1S/C19H26O7/c1-10-5-6-18(8-23-11(2)20)13(7-10)26-16-14(22)15(25-12(3)21)17

InchiKey: AUGQEEXBDZWUJY-UHFFFAOYSA-N

Formula: C19H26O7

SMILES: CC(=O)OCC12CCC(C)=CC1OC1C(O)C(OC(C)=O)C2(C)C12CO2

Mol. weight [g/mol]: 366.41

CAS: 2270-40-8

Physical Properties

Property code	Value	Unit	Source
gf	-468.27	kJ/mol	Joback Method
hf	-1031.43	kJ/mol	Joback Method
hfus	44.08	kJ/mol	Joback Method
hvap	98.47	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.125		Crippen Method

mcvol	263.320	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	2421.00		NIST Webbook
rinpol	2426.00		NIST Webbook
tb	959.13	K	Joback Method
tc	1186.01	K	Joback Method
tf	699.15	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.87	J/mol×K	959.13	Joback Method
cpg	1000.15	J/mol×K	996.94	Joback Method
cpg	1029.47	J/mol×K	1034.76	Joback Method
cpg	1061.22	J/mol×K	1072.57	Joback Method
cpg	1095.79	J/mol×K	1110.38	Joback Method
cpg	1133.57	J/mol×K	1148.19	Joback Method
cpg	1174.96	J/mol×K	1186.01	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2270408&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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