Trichothec-9-ene-3,4,8,15-tetrol, 12,13-epoxy-, 15-acetate 8-(3-methylbutanoate), (3«alpha»,4«beta»,8«alpha»)-

Other names: Toxin HT 2

Trichothec-9-ene-3«alpha»,4«beta»,8«alpha»,15-tetrol, 12,13-epoxy-, 15-acetate 8-isovalerate

HT 2 Toxin

Mycotoxin HT 2

T-2, Toxin analog

12,13-Epoxytrichothec-9-ene-3-«alpha»,4-«beta»,8-«alpha»,15-tetrol 15-acetate 8-isovalerate

HT-2

15-Acetoxy-3,4-dihydroxy-8-(3-methylbutyryloxy)-12,13-epoxy-«delta»9-trichothecene

NSC 278571

Inchi: InChI=1S/C22H32O8/c1-11(2)6-16(24)29-14-8-21(9-27-13(4)23)15(7-12(14)3)30-19-17(2

InchiKey: PNKLMTPXERFKEN-UHFFFAOYSA-N

Formula: C22H32O8

SMILES: CC(=O)OCC12CC(OC(=O)CC(C)C)C(C)=CC1OC1C(O)C(O)C2(C)C12CO2

Mol. weight [g/mol]: 424.48

CAS: 26934-87-2

Physical Properties

Property code	Value	Unit	Source
gf	-589.98	kJ/mol	Joback Method
hf	-1271.20	kJ/mol	Joback Method
hfus	53.48	kJ/mol	Joback Method
hvap	121.13	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	1.122		Crippen Method
mcvol	311.460	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	2809.00		NIST Webbook
rinpol	2809.00		NIST Webbook
rinpol	2809.00		NIST Webbook
tb	1114.84	K	Joback Method
tc	1367.01	K	Joback Method
tf	774.54	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.12	J/mol×K	1114.84	Joback Method
cpg	1331.56	J/mol×K	1156.87	Joback Method
cpg	1380.27	J/mol×K	1198.90	Joback Method
cpg	1433.79	J/mol×K	1240.92	Joback Method
cpg	1492.68	J/mol×K	1282.95	Joback Method
cpg	1557.46	J/mol×K	1324.98	Joback Method
cpg	1628.70	J/mol×K	1367.01	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C26934872&Units=SI

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