T-2 Mycotoxin

Other names: Trichothec-9-ene-3,4,8,15-tetrol, 12,13-epoxy-, 4,15-diacetate 8-(3-methylbutanoate), (3«alpha»,4«beta»,8«alpha»)-
Trichothec-9-ene-3«alpha»,4«beta»,8«alpha»,15-tetrol, 12,13-epoxy-, 4,15-diacetate 8-isovalerate
Fusariotoxin T 2
Insariotoxin
T 2 Toxin
Toxin T 2
Scirpenol, 8-(3-methylbutyryloxy)-diacetoxy-
3«alpha»-Hydroxy-4«beta»,15-diacetoxy-8«alpha»(3-methylbutyryloxy)-12,13-epoxy-trich
8-(3-Methylbutyryloxy)diacetoxyscirpenol
4«beta»,15-Diacetoxy-8«alpha»-(3-methylbutyryloxy)-3«alpha»-hydroxy-12,13-epoxytrich
8«alpha»-(3-Methylbutyryloxy)-4«beta»,15-diacetoxyscirp-9-en-3«alpha»-ol
Mycotoxin T 2
NSC 138780
(3«alpha»,4«beta»,8«alpha»)-12,13-epoxytrichothec-9-ene-3,4,8,15-tetrol 4,15-diacetate 8-(3-methylbutyrate)

Inchi: InChI=1S/C24H34O9/c1-11(2)7-17(27)33-20-12(3)8-16-18(15(20)9-29-13(4)25)23(6)21(3

InchiKey: SSHHYBPAMCLKRH-UHFFFAOYSA-N

Formula: C24H34O9

SMILES: CC(=O)OCC1C(OC(=O)CC(C)C)C(C)=CC2OC3C(O)C(OC(C)=O)C(C)(C21)C31CO1

Mol. weight [g/mol]: 466.52

CAS: 21259-20-1

Physical Properties

Property code	Value	Unit	Source
gf	-672.46	kJ/mol	Joback Method
hf	-1440.63	kJ/mol	Joback Method
hfus	64.73	kJ/mol	Joback Method
hvap	118.90	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	1.549		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
rinpol	3135.00		NIST Webbook
tb	1139.80	K	Joback Method
tc	1398.27	K	Joback Method
tf	780.28	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.39	J/mol×K	1139.80	Joback Method
cpg	1415.02	J/mol×K	1182.88	Joback Method
cpg	1452.91	J/mol×K	1225.96	Joback Method
cpg	1493.47	J/mol×K	1269.04	Joback Method
cpg	1537.10	J/mol×K	1312.11	Joback Method
cpg	1584.20	J/mol×K	1355.19	Joback Method
cpg	1635.19	J/mol×K	1398.27	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=C21259201&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

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