

Trichothec-9-en-8-one, 4-(acetyloxy)-12,13-epoxy-3,7,15-trihydroxy-, (3«alpha»,4«beta»,7«beta»)-

Other names: Trichothec-9-en-8-one 12,13-epoxy-3«alpha»,4«beta»,7«beta»,15-tetrahydroxy-,
Fusarenon X

Fusarenone X

Fusarenon

Inchi: InChI=1S/C17H22O8/c1-7-4-9-16(5-18,12(22)10(7)20)15(3)13(24-8(2)19)11(21)14(25-9)

InchiKey: XGCUCFKWVIWWNW-UHFFFAOYSA-N

Formula: C17H22O8

SMILES: CC(=O)OC1C(O)C2OC3C=C(C)C(=O)C(O)C3(CO)C1(C)C21CO1

Mol. weight [g/mol]: 354.35

CAS: 23255-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-655.13	kJ/mol	Joback Method
hf	-1207.85	kJ/mol	Joback Method
hfus	44.87	kJ/mol	Joback Method
hvap	122.16	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	-1.296		Crippen Method
mcvol	241.010	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	2485.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2485.00		NIST Webbook
tb	1084.59	K	Joback Method
tc	1328.00	K	Joback Method
tf	790.07	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.12	J/mol×K	1084.59	Joback Method
cpg	1037.63	J/mol×K	1125.16	Joback Method

cpg	1077.83	J/mol×K	1165.73	Joback Method
cpg	1122.16	J/mol×K	1206.30	Joback Method
cpg	1171.08	J/mol×K	1246.86	Joback Method
cpg	1225.03	J/mol×K	1287.43	Joback Method
cpg	1284.47	J/mol×K	1328.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23255698&Units=SI
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

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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