

Trichothec-9-ene-3-«alpha»,4-«beta»,8-«alpha»,15

Other names:

12,13-epoxy-, 3,4,15-triacetate,8-isovalerate

Acetyl-T-2

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

3,4,15-triacetate 8-isovalerate

T-2 Acetate

Acetyl-T-2-toxin

T-2 Toxin, acetyl

Inchi: InChI=1S/C26H36O10/c1-13(2)8-20(30)35-18-10-25(11-31-15(4)27)19(9-14(18)3)36-23-

InchiKey: NOTOVTQRFFVBSB-UHFFFAOYSA-N

Formula: C26H36O10

SMILES: CC(=O)OCC12CC(OC(=O)CC(C)C)C(C)=CC1OC1C(OC(C)=O)C(OC(C)=O)C2(C)C12C

Mol. weight [g/mol]: 508.56

CAS: 21259-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-750.50	kJ/mol	Joback Method
hf	-1538.90	kJ/mol	Joback Method
hfus	61.24	kJ/mol	Joback Method
hvap	114.99	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.263		Crippen Method
mcvol	370.960	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
tb	1174.58	K	Joback Method
tc	1439.14	K	Joback Method
tf	842.30	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1535.33	J/molxK	1174.58	Joback Method
cpg	1586.28	J/molxK	1218.67	Joback Method
cpg	1641.79	J/molxK	1262.77	Joback Method
cpg	1702.44	J/molxK	1306.86	Joback Method

cpg	1768.81	J/mol×K	1350.96	Joback Method
cpg	1841.48	J/mol×K	1395.05	Joback Method
cpg	1921.02	J/mol×K	1439.14	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=C21259212&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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