

Deoxynivalenol

Other names:	Trichothec-9-en-8-one, 12,13-epoxy-3,7,15-trihydroxy-, (3«alpha»,7«alpha»)-Vomitoxin Spiro[2,5-methano-1-benzoxepin-10,2'-oxirane], trichothec-9-en-8-one deriv. 12,13-Epoxy-3«alpha»,7«alpha»,15-trihydroxy-9-trichothecen-8-one 4-Deoxynivalenol 3«alpha»,7«alpha»,15-Trihydroxy-12,13-epoxytrichothec-9-en-8-one
Inchi:	InChI=1S/C15H20O6/c1-7-3-9-14(5-16,11(19)10(7)18)13(2)4-8(17)12(21-9)15(13)6-20-1
InchiKey:	LINOMUASTDIRTM-WHNKEALZSA-N
Formula:	C15H20O6
SMILES:	<chem>CC1=CC2OC3C(O)CC(C)(C34CO4)C2(CO)C(O)C1=O</chem>
Mol. weight [g/mol]:	296.32
CAS:	51481-10-8

Physical Properties

Property code	Value	Unit	Source
gf	-430.34	kJ/mol	Joback Method
hf	-901.43	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	108.86	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	-0.838		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		NIST Webbook
rinpol	2287.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	967.21	K	Joback Method
tc	1189.59	K	Joback Method
tf	699.61	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.54	J/mol×K	967.21	Joback Method
cpg	820.50	J/mol×K	1004.27	Joback Method
cpg	847.78	J/mol×K	1041.34	Joback Method
cpg	877.72	J/mol×K	1078.40	Joback Method
cpg	910.71	J/mol×K	1115.46	Joback Method
cpg	947.11	J/mol×K	1152.53	Joback Method
cpg	987.27	J/mol×K	1189.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51481108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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