T-2 Tetraol

Other names: Trichothec-9-ene-3,4,8,15-tetrol, 12,13-epoxy-, (3«alpha»,4«beta»,8«alpha»)-
Trichothec-9-ene-3«alpha»,4«beta»,8«alpha»,15-tetrol, 12,13-epoxy-
T-2 Tetraol toxin
T-2 toxin tetraol
Inchi: InChI=1S/C15H22O6/c1-7-3-9-14(5-16,4-8(7)17)13(2)11(19)10(18)12(21-9)15(13)6-20-1
InchiKey: ZAXZBJSXSOISTF-UHFFFAOYSA-N
Formula: C15H22O6
SMILES: CC1=CC2OC3C(O)C(O)C(C)(C2(CO)CC1O)C31CO1
Mol. weight [g/mol]: 298.33
CAS: 34114-99-3

Physical Properties

Property code	Value	Unit	Source
gf	-452.28	kJ/mol	Joback Method
hf	-936.30	kJ/mol	Joback Method
hfus	41.48	kJ/mol	Joback Method
hvap	120.98	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	-1.046		Crippen Method
mcvol	209.690	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	2547.00		NIST Webbook
tb	986.90	K	Joback Method
tc	1208.26	K	Joback Method
tf	687.97	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.46	J/mol×K	986.90	Joback Method
cpg	861.31	J/mol×K	1023.79	Joback Method
cpg	890.82	J/mol×K	1060.69	Joback Method
cpg	923.41	J/mol×K	1097.58	Joback Method

cpg	959.44	J/mol×K	1134.47	Joback Method
cpg	999.30	J/mol×K	1171.37	Joback Method
cpg	1043.40	J/mol×K	1208.26	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=C34114993&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