ACETYL-T-2-TOXIN

Other names:	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

Physical Properties

Property code	Value	Unit	Source
hfus	61.24	kJ/mol	Joback Method
logp	2.263		Crippen Method
mcvol	370.960	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1535.33	J/mol×K	1174.58	Joback Method
cpg	1586.28	J/mol×K	1218.67	Joback Method
cpg	1641.79	J/mol×K	1262.77	Joback Method
cpg	1702.44	J/mol×K	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: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21259212&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume