MONOACETOXYSCIRPENOL

Other names:	(3«alpha»)-12,13-Epoxytrichothec-9-ene-3,4,15-triol 15-acetate
	Trichothec-9-ene-3«alpha»,4«beta»,15-triol, 12,13-epoxy-, 15-acetate
	Trichothec-9-ene-3,4,15-triol, 12,13-epoxy-, 15-acetate, (3«alpha»,4«beta»)-
	15-Acetoxyscirpenol
	Deacetylanguidin
	15-MAS
	Monoacetoxyscirpenol
	15-Acetoxyscirpen-3,4-diol
	15-Acetylscirpenetriol
	15-Mono-O-acetylscirpenol
	15-O-Acetylscirpenetriol
	4-Deacetylanguidin
	NSC 267030
	Scirp-9-ene-3«alpha»,4«beta»,15-triol, 12,13-epoxy-, 15-acetate
	15-Acetoxyscripenol
Inchi:	InChI=1S/C17H24O6/c1-9-4-5-16(7-21-10(2)18)11(6-9)23-14-12(19)13(20)15(16,3)17(14
InchiKey:	IRXDUBNENLKYTC-UHFFFAOYSA-N
Formula:	C17H24O6
SMILES:	CC(=O)OCC12CCC(C)=CC1OC1C(O)C(O)C2(C)C12CO2
Mol. weight [g/mol]:	324.37

Physical Properties

Property code	Value	Unit	Source
hfus	40.20	kJ/mol	Joback Method
logp	0.554		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.22	J/mol×K	929.26	Joback Method
cpg	886.17	J/mol×K	965.68	Joback Method

cpg	911.95	J/mol×K	1002.10	Joback Method
cpg	939.94	J/mol×K	1038.52	Joback Method
cpg	970.50	J/mol×K	1074.94	Joback Method
cpg	1003.99	J/mol×K	1111.36	Joback Method
cpg	1040.77	J/mol×K	1147.78	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2623225&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

hfus: Enthalpy of fusion at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices