Furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-6(5aH)-on
5,8,8a,9-tetrahydro-5-(3,4,5-trimethoxyphenyl)-, [5R-(5«alpha»,5a«beta»,8a«alpha»)]-

Othernames:	Podophyllotoxin, deoxy- Anthrien Deoxypodophyllotoxin Desoxypodophyllotoxin Hernandion Silicicolin Hernandin 5-(3,4,5-Trimethoxyphenyl)-5,8,8a,9-tetrahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol-6(5 (-)-Anthricin (5R,5aR,8aR)- (-)-Deoxypodophyllotoxin (-)-Desoxypodophyllotoxin 4-Deoxypodophyllotoxin AS 2-3 Furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-6(5aH)-one, 5,8,8a,9-tetrahydro-5-(3,4,5-trimethoxyphenyl)-, (5R,5aR,8aR)- (5R,5aR,8aR)-5-(3,4,5-Trimethoxyphenyl)-5,5a,8a,9-tetrahydrofuro[3',4':6,7]naphtho[2,3-
Inchi:	InChI=1S/C22H22O7/c1-24-17-6-12(7-18(25-2)21(17)26-3)19-14-8-16-15(28-10-29-16)5
InchiKey:	ZGLXUQQMLLIKAN-UHFFFAOYSA-N
Formula:	C22H22O7
SMILES:	COc1cc(C2c3cc4c(cc3CC3COC(=O)C32)OCO4)cc(OC)c1OC
Mol. weight [g/mol]:	398.41
CAS:	19186-35-7

Physical Properties

Property code	Value	Unit	Source
gf	-224.40	kJ/mol	Joback Method
hf	-811.29	kJ/mol	Joback Method
hfus	57.80	kJ/mol	Joback Method
hvap	98.01	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	2.918		Crippen Method
mcvol	277.530	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	3267.50		NIST Webbook
tb	1026.42	K	Joback Method
tc	1278.49	K	Joback Method
tf	730.58	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.08	J/mol×K	1026.42	Joback Method
cpg	974.83	J/mol×K	1068.43	Joback Method
cpg	985.98	J/mol×K	1110.44	Joback Method
cpg	995.57	J/mol×K	1152.46	Joback Method
cpg	1003.66	J/mol×K	1194.47	Joback Method
cpg	1010.31	J/mol×K	1236.48	Joback Method
cpg	1015.55	J/mol×K	1278.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19186357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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