PACLITAXEL

Other names:	7,11-Methano-5H-cyclodeca(3,4)benz(1,2-b)oxete, benzenepropanoic acid deriv.
	Benzenepropanoic acid, «beta»-(benzoylamino)-«alpha»-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca(3,4)benz(1,2-b)oxet-9-yl ester, (2aR-(2a«alpha»,4«beta»,4a«beta»,6«beta»,9«alpha»(«alpha»R*,«beta»S*),11«alpha»,12«alpha»,12a«alpha»,12b«alpha»))-
	Benzenepropanoic acid, «beta»-(benzoylamino)-«alpha»-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca(3,4)benz(1,2-b)oxet-9-yl ester, (2aR-(2a«alpha»,4«beta»,4a«beta»,6«beta»,9«alpha»(«alpha»R*,«beta»S*),11«alpha»,12«alpha»,12a«alpha»,12b«alpha»))-
	(2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca(3,4)benz(1,2-b)oxet-9-yl ester, benzenepropanoic acid, «beta»-(benzoylamino)-«alpha»-hydroxy-, (2aR-(2a«alpha»,4«beta»,4a«beta»,6«beta»,9«alpha»(«alpha»R*,«beta»S*),11«alpha»,12«alpha»,12a«alpha»,12b«alpha»))-
	Cissus quadrangularis extract
	NSC-125973
	Tax-11-en-9-one, 5«beta»,20-epoxy-1,2«alpha»,4,7«beta»,10«beta»,13«alpha»-hexahydroxy-, 4,10-diacetate 2-benzoate, 13-ester with (2R,3S)-N-benzoyl-3-phenylisoserine
	taxol
Inchi:	InChI=1S/C47H51NO14/c1-25-31(60-43(56)36(52)35(28-16-10-7-11-17-28)48-41(54)29-
InchiKey:	RCINICONZNJXQF-UHFFFAOYSA-N
Formula:	C47H51NO14
SMILES:	CC(=O)OC1C(=O)C2(C)C(O)CC3OCC3(OC(C)=O)C2C(OC(=O)c2ccccc2)C2(O)CC(OC(
Mol. weight [g/mol]:	853.92

Physical Properties

Property code	Value	Unit	Source
hfus	93.88	kJ/mol	Joback Method
log10ws	-3.52		Aqueous Solubility Prediction Method
logp	3.736		Crippen Method
mcvol	620.430	ml/mol	McGowan Method
tf	488.15	K	Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide
tf	487.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	6262.61	J/mol×K	2164.80	Joback Method
cpg	8832.72	J/mol×K	2436.77	Joback Method
cpg	12394.69	J/mol×K	2708.73	Joback Method
cpg	17129.84	J/mol×K	2980.70	Joback Method
cpg	23219.50	J/mol×K	3252.67	Joback Method

cpg	30844.99	J/mol×K	3524.63	Joback Method
cpg	40187.62	J/mol×K	3796.60	Joback Method

Sources

Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je049551l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33069624&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point