

Paclitaxel

Other names:

7,11-Methano-5H-cyclodeca(3,4)benz(1,2-b)oxete, benzenepropanoic acid deriv.

[illegible][illegible]

Inchi:

(2R,3S)-5-(benzoyl-3-gluceryl-iso-serine-43(56)36(52)35(28-16-10-7-11-17-28)48-41(54)29-

InchiKey:

RCINICONZNJXOF-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]:

853.91

CAS:

33069-62-4

Physical Properties

Property code	Value	Unit	Source
hf	-1865.61	kJ/mol	Joback Method
hvap	237.43	kJ/mol	Joback Method
log10ws	-3.52		Aqueous Solubility Prediction Method
logp	4.310		Crippen Method
mcvol	620.430	ml/mol	McGowan Method
pc	767.34	kPa	Joback Method
tb	2229.50	K	Joback Method
tc	4248.49	K	Joback Method
tf	487.65	K	Aqueous Solubility Prediction Method
tf	488.15	K	Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33069624&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/jc0049551l

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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