

thujaplicin

Other names:	«alpha»-thujaplicin
Inchi:	InChI=1S/C10H12O2/c1-7(2)8-5-3-4-6-9(11)10(8)12/h3-7H,1-2H3,(H,11,12)
InchiKey:	TUFYVOCKVJOUIR-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	<chem>CC(C)c1cccc(O)c1=O</chem>
Mol. weight [g/mol]:	164.20
CAS:	1946-74-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.63		Crippen Method
logp	1.876		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
rinpol	1411.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1400.00		NIST Webbook
ripol	2120.00		NIST Webbook
ripol	2120.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1946743&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices

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