

Solanidan-3-ol, (3«beta»,5«alpha»)-

Other names:	(22R,25S)-5«alpha»-Solani-dan-3«beta»-ol Demissidin Demissidine 22R,25S-5«alpha»-Solani-danine-3«beta»-ol 5«alpha»-Solani-dan-3«beta»-ol 5«alpha»-Solani-dan-3«beta»-ol, (22R,25S)- (22S,25S)-5-«alpha»-Solani-danine-3-«beta»-ol (22S,25S)-5-«alpha»-Solani-dan-3-«beta»-ol
Inchi:	InChI=1S/C27H45NO/c1-16-5-8-23-17(2)25-24(28(23)15-16)14-22-20-7-6-18-13-19(29)9
InchiKey:	JALVTHFTYRPDMB-ICOJOGTOSA-N
Formula:	C27H45NO
SMILES:	CC1CCC2C(C)C3C(CC4C5CCC6CC(O)CCC6(C)C5CCC43C)N2C1
Mol. weight [g/mol]:	399.65
CAS:	474-08-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	5.735		Crippen Method
mcvol	341.980	ml/mol	McGowan Method
rinpol	3137.00		NIST Webbook
rinpol	3137.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C474088&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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