

Solanid-5-en-3-ol, (3«beta»)-

Other names:	Solanid-5-en-3«beta»-ol Solanidin Solanidine Solatubin Solatubine 22R,25S-Solanidanine 3«beta»-Solanid-5-en-3-ol NSC 76025
Inchi:	InChI=1S/C27H43NO/c1-16-5-8-23-17(2)25-24(28(23)15-16)14-22-20-7-6-18-13-19(29)9
InchiKey:	JVKYZPBMZPJNAJ-ICPPQKBESA-N
Formula:	C27H43NO
SMILES:	CC1CCC2C(C)C3C(CC4C5CC=C6CC(O)CCC6(C)C5CCC43C)N2C1
Mol. weight [g/mol]:	397.64
CAS:	80-78-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.58		Crippen Method
logp	5.655		Crippen Method
mcvol	337.680	ml/mol	McGowan Method
rinpol	3130.00		NIST Webbook
rinpol	3129.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C80784&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

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