

Solanthrene

Inchi: InChI=1S/C27H43N/c1-17-8-11-23-18(2)25-24(28(23)16-17)15-22-20-10-9-19-7-5-6-13-2
InchiKey: HKIXEELHOHFWNE-QYZUSCGHSA-N
Formula: C27H43N
SMILES: CC1CCC2C(C)C3C(CC4C5CC=C6CCCCC6(C)C5CCC43C)N2C1
Mol. weight [g/mol]: 381.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.21		Crippen Method
logp	6.684		Crippen Method
mcvol	331.810	ml/mol	McGowan Method
rinpol	2942.00		NIST Webbook
rinpol	2942.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R27904&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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<https://www.cheméo.com/cid/62-602-4/Solanthrene.pdf>

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