homo-6-epipodopetaline

Inchi: InChI=1S/C21H33N3/c1-3-9-22-14-21-13-17(18(22)7-1)12-16-6-5-11-24(20(16)21)15-23-
InchiKey: PKBPMASMWALHEP-ALAWOQLPSA-N
Formula: C21H33N3
SMILES: C1=C2CCCN3CN4CCCCC4C4(CC1C1CCCCN1C4)C23
Mol. weight [g/mol]: 327.51
CAS: 114370-18-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	3.077		Crippen Method
mcvol	267.230	ml/mol	McGowan Method
rinpol	2562.00		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=C114370182&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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